MEASURES FOR HARTREE-FOCK STATES AND HAMILTONIAN OPERATORS AND A NEW VARIATIONAL METHOD IN THE STUDY OF NUCLEI

BY

SATYAN VENKATARAMIAH

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AHMEDABAD 380 009

INDIA

DEDICATED

TO MY PARENTS

CERTIFICATE

I hereby declare that the work presented in this thesis is original and has not formed the basis for the award of any degree or diploma by any University or Institution.

Certified:

Jitendra C. Parikh
(Professor-in-Charge)
October 4, 1976.

V. Satyan
Satyan Venkataramaiah
(Author)

S T A T E M E N T

We describe in this thesis our study of goodness of Hartree-Fock states and also the development and application of a variational method based on the minimization of energy variance for obtaining Slater determinants. We also describe here our study of the decomposition of fermion operators under unitary groups and norms of these operators in spectroscopic spaces, our main object here being the investigation of questions relating to the efficiency of the HF procedure in generating an effective one-body operator from the given two-body interaction.

We have studied the 'goodness' of Hartree-Fock (HF) states by evaluating their widths. The width provides us with a measure of departure of an approximate wave function from the 'exact' solution of the Hamiltonian in the model space. We have done radial Hartree-Fock and width calculations for some light spherical nuclei in the model space of first four oscillator major shells using three different sets of realistic two-body interactions. We find that the widths are large for the HF solutions of these nuclei. These large values for widths imply that the

ground state wave functions of these nuclei cannot be described by single Slater determinants. We have also evaluated the second order perturbation correction to the HF energy and also the intensity of the HF wave function in the wave function corrected to first order. We find the corrections to the energy and the wave function to be appreciable for the nuclei studied. This implies that the correlation effects are important and hence they cannot be ignored. We have also studied the goodness of deformed HF wave functions. We present here our results for widths of N=Z even-even nuclei calculated in the 0d-1s major shell using a schematic interaction, the Preedom-Wildenthal and also the K+12FP interactions.

We have also developed a variational method for obtaining Slater determinantal wave functions by minimizing the energy variance instead of energy as is done in the conventional HF variational procedure. The equations for determining the self-consistent set of single particle orbits using the new variational procedure have been derived. Using these equations Slater determinantal wave functions having minimum width have been obtained for some light spherical nuclei using three different sets of realistic two-body interactions. We have also estimated

the perturbation corrections for these new wave functions. Our results show that a minimum energy variance solution exists in the neighbourhood of the HF solution. Further, the minimum variance obtained is at best only a few percent smaller than the variance of the HF solution. This means that the wave function obtained by the minimization of variance is not really very different from the HF one. Thus for light spherical nuclei we find that HF solution nearly minimizes the width in the ground state region. We have also made a comparative study of the two different variational procedures from the standpoint of perturbation corrections and other physical properties.

The second major topic dealt with in this thesis is about the structure of fermion operators and spaces. We have studied here the question to what extent the HF procedure converts the two-body interaction into an effective one-body operator. For this purpose we require two things. First, we need a proper classification scheme for operators in which we can carry out an orthogonal decomposition of them. Secondly, we need proper measures or norms for the sizes of operators so that we can study their behaviour in spectroscopic spaces and also make a comparative study of them. In our study we have used the group theoretic classification for operators the relevant

groups being unitary groups in spectroscopic spaces. More precisely, we have here a set of N single-particle states in which m particles are distributed. We have classified the two-body interaction according to the irreducible symmetries of the unitary group U(N) and its direct sum subgroup $U(m)\dot{+}U(N-m)$. The subgroup here is the one generated by the HF decomposition of s.p. space into m occupied and (N-m) unoccupied states. We have studied here the question to what extent the irreducible tensor part of the two-body interaction H(2) under U(N) is converted into an effective one-body operator under the subgroup $U(m)\dot{+}U(N-m)$ supplied by the HF procedure. As already said, for our purpose we need also suitable norms for the sizes of operators in m particle spaces. We have used here the Euclidean norm as a proper measure for the size of an operator. We have derived a polynomial expression for the square of the norm of the effective one-body operator which results when the two-body interaction is classified under the subgroup generated by the HF procedure. Next a quantity called conversion ratio is defined in terms of norms of different symmetry parts of the interaction decomposed according to U(N) and $U(m)\dot{+}U(N-m)$. This ratio tells us to what extent

the two-body interaction has been converted into an effective one-body operator when a HF calculation is done. It further indicates in a global sense how good is the HF single-particle basis. This ratio has been evaluated for the HF solutions of some N=Z even even nuclei both in 0f-1p and 0d-1s shells using realistic two-body interactions. Our studies reveal that this conversion is quite small which implies that a large part of the two-body interaction is still irreducible under the subgroup generated by the HF procedure and that the HF s.p. basis is not a good universal basis.

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CHAPTER I

INTRODUCTION

The nucleus is a system of finite number of fermions interacting through strong, short range forces. The number of nucleons in a given nucleus may be anywhere from a few to a few hundred. The internucleon force besides being strong and short ranged is also complex in nature having central, spin-orbit and tensor components and perhaps has also many-body character. Yet another aspect of this complicated force is its strong repulsive character at very short distances. It is not surprising then that one observes a rich and wide-ranging variety of phenomena in nuclei. From the theoretical viewpoint the understanding of and predicting the behaviour of a nucleus forms a fascinating, though at times difficult, study. The problem here is that of calculating all the properties of a finite many-body system of fermions interacting through a complicated, as yet not fully understood force. More precisely, on the one hand one has the problem of dealing with the complicated nuclear force whose exact nature is not known and on the other, the problem of solving the finite many-body Schroedinger equation. We are concerned in this thesis with approaches to the approximate solution of the latter problem.

The independent particle model (IPM) provides the simplest of all the approaches towards an approximate solution of the nuclear many-body Schroedinger equation. The IPM approach consists in taking the strongly interacting many-particle system to be a system of non-interacting particles moving in an average field. Depending upon how this average field is constructed there are many forms of IPM. A widely-used IPM is the Hartree-Fock (HF) method in which the average field generated is a self-consistent field giving minimum energy for the system. This HF self-consistent field idea is at the back of all the present-day microscopic theories of nuclear structure. These sophisticated theories start from HF as a first approximation and attempt in different ways to include the residual interaction which is ignored in the HF picture. This thesis is concerned with the 'goodness' of wave function and operators obtained by the HF method.

The approximate wave function used for nucleons in the IPM is a Slater determinant which is an antisymmetrized product of independent particle wave functions. In the last ten years or so, such a determinant has very often been obtained by the HF method[1-4] in which one finds the determinant having the lowest energy. It is generally accepted that the HF approximation describes many nuclear properties,

including the ground state energy well. In particular some of the single-particle properties (expectation values of one-body operators in the HF state) show spectacular agreement[4] with experiments. In spite of the agreement one finds with the experiment it is not clear how 'good' the HF wave function is. To be more precise, one does not know how well this approximate wave function compares with the "exact" solution of the Hamiltonian in the model space. Often one also does not know how the calculated properties would change with improvement in the wave function. It seems justified therefore not to strive for "very good" agreement between the HF results and the experimental ones without a proper investigation of corrections to the HF. In view of this, we make a modest beginning in chapter II of systematically studying these questions. A more detailed discussion of some measures for testing approximate wave functions and the related variational principles is given in the same chapter.

Consider the HF solution for the nuclear system and evaluate its variance[5] $\sigma^2 = \langle H^2 \rangle - \langle H \rangle^2$. The width σ provides us with a measure of departure of the approximate wave function from the "exact" solution for the system. Of course this quantity by itself does not tell us how important the "correlation" effects are for the nuclear properties.

One way of learning about these is to improve the wave function by the use of perturbation theory. We have therefore evaluated the correction to the HF wave function and the HF energy in perturbation theory. This is described in chapter II. The width may also be used as a measure for comparing two approximate wave functions. For example, given the widths of two determinantal states, one can say that the one with the smaller width is closer to the "exact" solution of the system. In the same chapter we also discuss how the width of the HF state changes with a change in the size of the vector spaces. We also examine the changes in the ground state energy with this truncation and see how the width is related to the total energy spectrum span of the nuclear system.

Besides studying the HF solution we also examine in chapter III an alternative variational procedure suggested earlier[6] to obtain determinantal states. In this we minimize the variance σ^2 for the system rather than the energy. It should be clear that the energy of the new determinant Ψ_σ will be higher than that of Ψ_{HF} but its width will be smaller. If we therefore use the width as a measure of "goodness" of a wave function then the state Ψ_σ is an improvement over Ψ_{HF}. Moreover, if we carry out perturbation theory corrections for Ψ_σ and Ψ_{HF} we expect

smaller 2ph correction for Ψ_σ than for Ψ_{HF}. This is because in the determination of Ψ_σ we are already including some excitations to intermediate 2ph states. Of course as far as the energy criterion is concerned the HF solution is superior to the corresponding solution obtained by minimizing σ^2.

The numerical calculation in chapter III are carried out for light "spherical" nuclei within the space of three and four harmonic oscillator shells. Three different effective interactions have been used. It should be pointed out that the calculations we have carried out are meant for "internal" comparison of the two variational methods and for illustrating the various points. It is not our aim to compare the results of our calculations with experimental quantities.

In chapter IV we extend our study of goodness of approximate wave functions to the class of deformed HF wave functions. Results for widths of N=Z even even nuclei calculated in the 0d-1s major shell using two different realistic two-body interactions are given. We also describe a schematic interaction in 0d-1s shell and give results for this interaction.

Another major topic dealt with in this thesis is concerned with the properties of fermion operators and

spaces. This is described in chapter V. Our main object here is to study the efficiency with which the two-body interaction is converted into an effective one-body operator by the HF "machinery". This efficiency factor indicates in a global sense how good is the HF single-particle basis. If a large part of the two-body interaction gets converted into a one-body like operator under HF then we can say that the Hamiltonian behaves essentially like a (0+1)-body operator and that the s.p. basis generated by the HF procedure is on the whole a good basis. One can also use this criterion for goodness of s.p. basis to seek the best s.p. basis which would be the one which optimizes this contribution from two-body term to an effective one-body term. The formulation and investigation of these and other related questions involve the use of a mathematical framework in which one carries out orthogonal decomposition of operators. Further, one needs measures for the sizes of operators so that one can study their behaviour in many particle spaces. The framework we use here for the classification of operators is that provided by unitary groups in spectroscopic spaces. As a measure for the size of an operator we make use of the Euclidean norm of an operator[7].

We all know that for the most part of the current microscopic theories of nuclear structure are attempts to solve

the finite many-body problem in truncated spaces defined by a finite number N of single-particle states. With the consideration of unitary transformations in these finite spaces the unitary group in N-dimensions viz.U(N) automatically enters into the discussion forming a starting point for all further group theoretic discussions of nuclear structure. Thus the unitary group U(N) and also its family of subgroups provide a natural and convenient mathematical framework for the study of the structure of fermion operators and spaces and also for investigating other physically relevant questions about them. We use this framework here to study the goodness of HF s.p. basis. The relevant groups here are the unitary group U(N) and its family of direct sum subgroups $U(m)\dot{+}U(N-m)$ where N is the total number of s.p.states and m is the number of particles. The subgroup we discuss here is the one generated by the HF procedure in which one decomposes via a variational procedure the N s.p.states into m occupied and (N-m) unoccupied ones. We decompose the interaction into its irreducible representations under both the U(N) and $U(m)\dot{+}U(N-m)$ groups using the standard techniques for the unitary group decomposition of a general fermion operator. We describe these techniques in detail[8-10]. Further we need proper measures for the sizes of operators and their symmetry parts to study their relative importance. The measure we

consider here is the Euclidean norm of an operator. We derive an expression for the square of the norm of total (0+1)-unitary rank part of the interaction when decomposed under the group $U(m)\dot{+}U(N-m)$. In terms of this norm and also the norms of various irreducible parts of H under U(N) we define a ratio R which serves as a global measure for the goodness of the HF s.p.basis[9]. This ratio tells us how much of the two-body interaction has been converted into an effective one-body operator when a HF calculation is done. We present the results of norms of various parts of the interaction decomposed under U(N) and $U(m)\dot{+}U(N-m)$ along with a discussion of them for N=Z even even nuclei in 0f-1p and 0d-1s shells using realistic two-body interactions. We also evaluate the efficiency ratio R for these nuclei.

Finally in Chapter VI we present a summary of the entire work and also some suggestions for future research.

REFERENCES FOR CHAPTER I

1. N. Ullah and R.K. Nesbet, Nucl. Phys. 39, 239 (1962); Phys. Rev. 134B, 308 (1964).
   A.K. Kerman, J.P. Svenne, F.M.H. Villars, Phys.Rev. 147, 710 (1966).
2. G. Ripka, Advances in Nuclear Physics, edited by M. Baranger and E. Vogt (Plenum Press, New York, 1968), Vol.I, Chap.3.
3. R.M. Tarbutton and K.T.R. Davies, Nucl.Phys.A120, 1 (1968).
4. J.W. Negele, Phys. Rev. C1, 1260 (1970).
5. J.C. Parikh and J.P. Svenne, Phys. Rev. C6, 34 (1972).
6. K.H. Bhatt and J.C. Parikh, Phys. Letts.44B, 338(1973).
7. J.B. French, Phys.Letts. 26B, 75 (1967).
8. F.S. Chang, J.B. French and T.H. Thio, Annals of Physics, 66, 137 (1971).
   J.C. Parikh, 'Group Symmetries in Nuclear Structure' to appear in Advances in Nuclear Physics, edited by M. Baranger and E. Vogt (Plenum Press, New York).
9. F.S. Chang, Thesis, University of Rochester (1970).
10. C.M. Vincent, Phys. Rev. 163, 1044 (1967).

CHAPTER II

MEASURES FOR DETERMINANTAL WAVE FUNCTIONS AND CORRESPONDING VARIATIONAL PROCEDURES

A. INTRODUCTION

We discuss in this section two measures for determining the "goodness" of an approximate wave function.

First we consider as a measure, the width σ of the approximate state which is defined through the variance σ^2. The variance σ^2 for a state $|\Psi\rangle$ is defined[1-4] to be

$$\sigma^2(\Psi) = \langle\Psi|H^2|\Psi\rangle - |\langle\Psi|H|\Psi\rangle|^2 \qquad \text{IIA(1)}$$

where H is the Hamiltonian of the system. It follows from this definition that, if $|\Psi\rangle$ is an exact eigenstate of H then its width σ is zero. Otherwise, $|\Psi\rangle$ will have a non-zero width which will give us a measure of the departure of $|\Psi\rangle$ from an eigenstate of H.

In order to get some more understanding of the quantity σ consider the expansion of $|\Psi\rangle$ over the complete set of eigenstates $|\Phi_k\rangle$ of our system. We have

$$|\Psi\rangle = \sum \alpha_k |\Phi_k\rangle$$

where α_k are the coefficients of expansion. A plot of the intensities $|\alpha_k|^2$ versus energy will then provide a picture of the way in which the state $|\Psi\rangle$ is distributed over the exact eigenstates of H. In practice we seldom know all the α_k's and E_k's and hence we will not be able to determine the distribution of $|\Psi\rangle$. Let us suppose however that we know the energy and the variance of $|\Psi\rangle$. These can be written as

$$E = \langle\Psi|H|\Psi\rangle = \sum_k |\alpha_k|^2 E_k$$

$$\sigma^2(\Psi) \equiv \mu_2 = \sum_k |\alpha_k|^2 E_k^2 - \left(\sum_k |\alpha_k|^2 E_k\right)^2 \qquad \text{IIA(2)}$$

We see from these equations that E is the mean energy and σ^2 the second central moment of the distribution - i.e. these are the lowest two moments of the distribution. As we evaluate higher central moments $\mu_p = \langle\Psi|(H-E)^p|\Psi\rangle \; (p>2)$ we learn more and more about the distribution. It should be clear therefore that after the energy the variance is the next simplest quantity that we can evaluate for a state $|\Psi\rangle$. Note that the energy of a state by itself gives no indication at all about the "goodness" of the wave function but the width does provide some information. In fact it gives the **spread** of $|\Psi\rangle$ over the exact eigenstates of H.

Further, the width can be used to give both a lower and an upper bound to an exact eigen energy of the system. More precisely, we have the relation

$$E-\sigma \leq \quad E_o \leqslant E+\sigma \qquad \text{IIA(3)}$$

where E and σ are the energy and the width of the approximate state $|\Psi\rangle$ and E_o is the exact eigen energy closest to E - i.e. $|E-E_o| < |E-E_k|$ for all E_k. This can be seen as follows: We have

$$\sigma^2(\Psi) = \sum_k \alpha_k^2 (E_k-E)^2 \qquad \text{IIA(4)}$$

and

$$\sum_k \alpha_k^2 = 1 \qquad \text{IIA(5)}$$

Since $\alpha_k^2 \geqslant 0$, $(E_k-E)^2 \geqslant 0$, we can replace the factors in Eq.IIA(4) by their smallest value $(E_o-E)^2$. Then using Eq.IIA(5) we get

$$\sigma^2 \geqslant (E_o-E)^2$$

from which it follows that

$$E-\sigma \leq \quad E_o \leqslant \quad E+\sigma$$

Thus if F is closest to the exact ground state energy then the lowest two moments provide bounds to the exact ground state energy.

Another possible measure which is often used is the overlap of the approximate state $|\Psi\rangle$ with the exact ground state wave function. This measure is generally very difficult if not impossible to evaluate. Thus this measure is available only in some restricted problems and hence has limited usefulness.

It is worthwhile recalling at this stage that, amongst variational solutions, the one with the lower energy does not necessarily have a smaller width or a larger overlap with the exact ground state wave function. Furthermore, a smaller width does not imply a larger overlap with the ground state wave function either. Thus the energy, the width and the overlap provide different criteria for discussing approximate wave functions.

Further, corresponding to each of these criteria one can set up a variational procedure. It should be evident that if we allow for the most general variation in the wave function then each procedure would be equivalent to solving the Schrodinger equation. It is when we put restrictions on the variational wave functions that we obtain different variational solutions. For determinantal states, the minimi-

zation of energy leads to the well-known Hartree-Fock (HF) method. The minimization of energy variance σ^2 for Slater determinants will be discussed in detail in chapter III. The optimization of overlap has been considered by Kelson and Shadmon[5].

In this chapter we consider the HF variational procedure and the evaluation of widths for HF states. This will be presented in the following six sections. First we describe the HF method in some detail and then specialize the method to case of double-closed shell nuclei and give the relevant expressions. In section D we discuss the centre of mass correction and also the perturbation corrections to the HF energy and wave function. Next in section E we describe in detail a method for evaluating widths of states and specialize it to the HF case. Numerical calculations for ^{4}He, ^{16}O and ^{40}Ca are described and the results discussed in section F. Finally in section G a study of the effect of enlarging the model space is described.

B. THE HARTREE-FOCK METHOD

There are already many articles[6-10] on the Hartree-Fock (HF) approximation and hence in this section we briefly discuss the method and give the relevant expressions.

If $|\Psi\rangle$ is a Slater determinant describing the state of an A particle system then we can write it in the occupation number representation as

$$|\Psi\rangle = \prod_{\alpha=1}^{A} a_\alpha^+ |0\rangle \qquad \text{IIB(1)}$$

where the operator a_α^+ creates a fermion in the orbit α and so on. These a_α^+'s and their corresponding destruction operators a_α's obey the well-known fermion anticommutation rules:

$$\begin{aligned} \left[a_p^+ , a_q^+\right]_+ &= 0 = \left[a_p , a_q\right]_+ \\ \left[a_p^+ , a_q\right]_+ &= \delta_{pq} \end{aligned} \qquad \text{IIB(2)}$$

In this representation the Hamiltonian H of the system can be written as

$$H = \sum_{pq} \langle p|t|q\rangle a_p^+ a_q + \frac{1}{4} \sum_{\substack{pq \\ p'q'}} \langle pq|V|p'q'\rangle a_p^+ a_q^+ a_{q'} a_{p'} \qquad \text{IIB(3)}$$

Here t is the kinetic energy operator $p^2/2m$, V is the two-body interaction operator and $\langle pq|\ V\ |\ rs\rangle$ is an anti-symmetrized matrix element of V. The single particle (s.p.) states p,q,r,s... belong to a complete orthonormal set.

Before we proceed further we describe the notation that will be used throughout this thesis. The occupied single particle states will be denoted by the Greek letters $\alpha, \beta, \gamma, \delta, \lambda, \cdots$ and the unoccupied states by $i,j,k,l,m,\ldots$. Any general s.p. state will be denoted by p or q. Each s.p. state label here stands for the set of s.p. state quantum numbers $(n,l,j,\frac{1}{2},m,\tau)$ where n is the radial quantum number, l,j are respectively the orbital and total angular momentum quantum numbers and m is the projection of j on the z-axis. The '$\frac{1}{2}$' here is the nucleon isospin and τ its third component. Henceforth we shall drop this '$\frac{1}{2}$' and keep only τ . Further, we shall compactly label the set $(l,j,\frac{1}{2})$ by the letter s. Thus $s \equiv (l,j,\frac{1}{2})$. For instance, s_α stands for $(l_\alpha \; j_\alpha \; \frac{1}{2}) \equiv (l,j,\frac{1}{2})_\alpha$. Dropping the '$\frac{1}{2}$' we shall sometimes write $s_\alpha \equiv (l_\alpha, j_\alpha) \equiv (lj)_\alpha$.

Now in the HF method the wave function $|\Psi\rangle$ is determined by first requiring

$$\delta \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = 0 \qquad \text{IIB(4)}$$

where δ denotes the most general variation of $|\Psi\rangle$. Then to keep $|\Psi\rangle$ normalized δ is limited to first order variations only by requiring

$$\delta \langle \Psi | H | \Psi \rangle = 0 \qquad \text{IIB(5)}$$

We can write this variation in $|\Psi\rangle$ as

$$\delta |\Psi\rangle = \eta\, a_k^+ a_\alpha |\Psi\rangle \qquad \text{IIB(6)}$$

where η is an infinitesimal. Now $|\Psi\rangle$ and its complex conjugate $\langle\Psi|$ can be varied independently and we choose to vary $\langle\Psi|$. Then substituting for H from Eq.IIB(3) in Eq.IIB(5) and doing some algebra we finally arrive at the following equations

$$\langle k|t|\alpha\rangle + \sum_{\lambda=1}^{A} \langle k\lambda|v|\alpha\lambda\rangle = 0; \quad \alpha \leq A, \; k > A \qquad \text{IIB(7)}$$

These are the well-known Hartree-Fock equations. Let us define a single particle operator

$$\tilde{\epsilon} = \sum_{pq} \left[\langle p|t|q\rangle + \sum_{\lambda=1}^{A} \langle p\lambda|v|q\lambda\rangle \right] a_p^+ a_q$$

IIB(8)

where p,q are arbitrary s.p. states. Then Eq.IIB(7) is equivalent to the condition that $\tilde{\epsilon}$ has no matrix elements between the occupied single particle states and the unoccupied ones, i.e.

$$\langle k|\tilde{\epsilon}|\alpha\rangle = 0. \qquad \text{IIB(9)}$$

This condition allows us to diagonalize $\tilde{\epsilon}$ in the space of occupied (or unoccupied) s.p. states only. This can be achieved by choosing a suitable linear combination of the occupied states $|\alpha\rangle$ such that $\tilde{\epsilon}$ becomes diagonal. Then Eq.IIB(9) can be written as:

$$\langle\alpha|\tilde{\epsilon}|\beta\rangle = \epsilon_\alpha \delta_{\alpha\beta}$$
$$\tilde{\epsilon}|\alpha\rangle = \epsilon_\alpha|\alpha\rangle \qquad \text{IIB(10)}$$

where ϵ_α's are eigenvalues of $\tilde{\epsilon}$. In practice, to solve the Hartree-Fock equations one expands the single-particle states $|\alpha\rangle$ in a convenient orthonormal complete set of wave functions $|i\rangle$ which are usually the harmonic oscillator wave functions. Thus

$$|\alpha\rangle = \sum_i C_i^\alpha |i\rangle \qquad \text{IIB(11)}$$

where C_i^α are the expansion coefficients. Using this in Eq.IIB(10) and also the orthonormality property of the basis set we get

$$\sum_j \langle j|\tilde{\epsilon}|i\rangle C_j^\alpha = \epsilon_\alpha C_i^\alpha \qquad \text{IIB(12)}$$

where

$$\langle j|\tilde{\epsilon}|i\rangle = \langle j|t|i\rangle + \sum_\alpha \langle j\alpha|v|i\alpha\rangle \qquad \text{IIB(13)}$$

It is clear from Eq.IIB(13) that $\tilde{\epsilon}$ is a functional of the occupied orbits $|\alpha\rangle$. Hence to solve Eq.IIB(12) one has to choose a trial set of C's, calculate the matrix $\tilde{\epsilon}$ in Eq.IIB(13) and diagonalize it to get a new set of C's. With this new set one repeats the above procedure and thus carries on an iterative procedure until the set of C's after diagonalization is the same as the one before diagonalization. The set of s.p.wave functions $|\alpha\rangle$ so obtained are said to be self-consistent. With these s.p. wave functions one constructs the HF determinantal wave function. Also one computes the HF energy using the following expression:

$$
\begin{aligned}
E_{HF} &= \langle \Psi | H | \Psi \rangle \\
&= \sum_{\alpha=1}^{A} \langle \alpha | t | \alpha \rangle + \sum_{\alpha,\beta=1}^{A} \langle \alpha\beta | v | \alpha\beta \rangle \\
&= \sum_{\alpha=1}^{A} \langle \alpha | \tilde{\epsilon} | \alpha \rangle - \frac{1}{2} \sum_{\alpha\beta} \langle \alpha\beta | v | \alpha\beta \rangle \\
&= \frac{1}{2} \left[\sum_{\alpha=1}^{A} \langle \alpha | t | \alpha \rangle + \sum_{\alpha=1}^{A} \langle \alpha | \tilde{\epsilon} | \alpha \rangle \right]
\end{aligned}
$$

IIB(14)

where α , β now refer to the HF s.p.orbits.

C. THE RADIAL HARTREE-FOCK APPROXIMATION

Since our purpose is to study the goodness of HF states of some light double-closed shell nuclei, it is now necessary to specialize the general equations of the previous section to the case of spherical nuclei.

The HF equations (see Eq.IIB(7)) are solved by the matrix method using a basis of harmonic oscillator wave functions. The single particle states χ_p are expanded in a finite series of oscillator wave functions Φ_q:

$$\chi_p = \sum_q c_q^p \Phi_q \qquad \text{IIC(1)}$$

The expansion coefficients c_q^p as well as the number of terms in the expansion and the oscillator length parameter

($b^2 = \hbar/m\omega$) are parameters to be determined by the HF procedure.

When the assumption of spherical symmetry for the HF state of the nucleus is made, J^2 and J_Z commute with $\tilde{\epsilon}$, and therefore the Hartree-Fock orbitals χ_p must be eigenstates of J^2 and J_Z. Thus the states χ_p can be characterized by the set of quantum numbers $|njm\rangle$. For χ_p to be rotationally invariant, all the m states for a given nj must be occupied which is the case for the double-closed shell nuclei we are considering. Further, for these nuclei the HF s.p. orbitals have time-reversal symmetry, good parity and charge invariance. With all these invariances for the HF orbitals the expansion coefficients C^p_q in Eq.IIC(1) are diagonal in angular momentum quantum numbers and are real. Hence the sum in Eq.IIC(1) is over principle quantum number only. Thus Eq.IIC(1) becomes

$$|l_p j_p m_p \tau_p\rangle = \sum_{n_p} C^p_{n_p} \; |n_p l_p j_p m_p \tau_p\rangle \qquad \text{IIC(2)}$$

where the sum is over the radial quantum number n_p. (Here p labels any general s.p.state, not a proton label). In our notation (see Sec.IIB) this becomes

$$|s_p m_p \tau_p\rangle = \sum_{n_p} C^p_{n_p} \; |n_p s_p m_p \tau_p\rangle \qquad \text{IIC(3)}$$

We now give the expression for the matrix elements of the HF s.p. Hamiltonian (Eq.IIB(8)) in the spherical harmonic oscillator basis. Since $\tilde{\epsilon}$ is spherically symmetric, we have

$$\langle s_p m_p \tau_p | \tilde{\epsilon} | s_{p'} m_{p'} \tau_{p'} \rangle \hat{\delta}_{pp'}$$

$$= \langle s_p m_p \tau_p | t | s_{p'} m_{p'} \tau_{p'} \rangle \hat{\delta}_{pp'}$$

$$+ \sum_{\substack{s_\lambda m_\lambda \\ \tau_\lambda}} \langle s_p m_p \tau_p, s_\lambda m_\lambda \tau_\lambda | V | s_{p'} m_{p'} \tau_{p'}, s_\lambda m_\lambda \tau_\lambda \rangle \hat{\delta}_{pp'}$$

IIC(4)

where the delta function $\hat{\delta}_{pp'} = \delta_{s_p s_{p'}} \delta_{m_p m_{p'}} \delta_{\tau_p \tau_{p'}}$ $= \delta_{\ell\ell'} \delta_{mm'} \delta_{\tau\tau'}$. Using Eq.IIC(3) for $|s_p m_p \tau_p\rangle$ in Eq.IIC(4) and remembering that the C's are linearly independent we obtain

$$\langle n_p s_p m_p \tau_p | \tilde{\epsilon} | n'_p s_p m_p \tau_p \rangle$$

$$= \langle n_p s_p m_p \tau_p | t | n'_p s_p m_p \tau_p \rangle$$

$$+ \sum_{\substack{s_\lambda m_\lambda \\ \tau_\lambda}} \langle n_p s_p m_p \tau_p, s_\lambda m_\lambda \tau_\lambda | V | n'_p s_p m_p \tau_p, s_\lambda m_\lambda \tau_\lambda \rangle$$

IIC(5)

Since the matrix elements of $\tilde{\epsilon}$, t and V do not depend on m_p, τ_p we sum them over in Eq. IIC(5) and obtain the expression for the matrix elements of $\tilde{\epsilon}$ between s.p. harmonic oscillator orbits differing only in the radial quantum number. Further, we expand $|s_\lambda\ m_\lambda\ \tau_\lambda\rangle$ using Eq. IIC(3) and carry out angular momentum coupling for the uncoupled matrix elements of V using Clebsch-Gordan algebra. We finally obtain

$$\langle n_p s_p | \tilde{\epsilon} | n'_p\ \ s_p \rangle$$

$$= \langle n_p s_p |\ t\ | n'_p s_p \rangle$$

$$+ \frac{1}{2(2j_p+1)} \sum_{\substack{s_\lambda n_\lambda n'_\lambda \\ J\ T}} (2T+1)(2J+1) \langle (n_p s_p, n_\lambda s_\lambda) | V | (n'_p s_p, n'_\lambda s_\lambda) \rangle_{JT} \times C^{\lambda *}_{n_\lambda} C^{\lambda}_{n'_\lambda} \qquad \text{IIC(6)}$$

Then for each spherical symmetry label $s_p \equiv (\ell_p j_p)$ the $\tilde{\epsilon}$ matrix is set up and diagonalized. This procedure is repeated until self-consistency in the s.p. wave functions is achieved. At the end of this iterative cycle the HF energy is computed using the following equation:

$$EHF = \langle \Psi_{HF} |\ H\ | \Psi_{HF} \rangle$$

$$= \frac{1}{2} \sum_{\lambda_\alpha n_\alpha n'_\alpha} 2(2j_\alpha+1) \left[\langle \lambda_\alpha n_\alpha | t | \lambda_\alpha n'_\alpha \rangle + \langle \lambda_\alpha n_\alpha | \tilde{E} | \lambda_\alpha n'_\alpha \rangle \right] C^{\alpha *}_{n_\alpha} C^{\alpha}_{n'_\alpha}$$

IIC(7)

Another quantity which is of interest to us is the root mean square radius (mass radius). The mean square radius is given by

$$\langle r^2 \rangle = \langle \Psi_{HF} | \frac{1}{A} \sum_{i=1}^{A} r_i^2 | \Psi_{HF} \rangle$$

$$= \frac{b^2}{A} \sum_{\lambda_\alpha n_\alpha n'_\alpha} 2(2j_\alpha+1) \langle \lambda_\alpha n_\alpha | r^2 | \lambda_\alpha n'_\alpha \rangle C^{\alpha *}_{n_\alpha} C^{\alpha}_{n'_\alpha}$$

IIC(8)

where $b = \sqrt{\frac{\hbar}{m\omega}}$ is the oscillator length parameter and A is the mass number.

D. CENTRE OF MASS MOTION AND PERTURBATION CORRECTIONS

We are concerned here with light spherical nuclei and therefore centre of mass motion (cmm) cannot be neglected and its effect on the HF wave function, energy and width

have to be properly taken care of. For a system of non - interacting fermions moving in an arbitrary potential well the problem of seperation of the relative and the centre of mass motions is yet an unsolved one. It is only when the potential well is of the harmonic type that one can write the total wave function as a product of the wave functions for the relative and the centre of mass motions and thus separate the spurious excited states from the real excited states. One does not as yet know how to carry out such a factorization for the case of HF wave function. However, one can make a correction in terms of energy if not in terms of wave function. This is done by subtracting out from the total Hamiltonian the centre of mass kinetic energy operator to get the intrinsic Hamiltonian. It should be noted that the positive cmm kinetic energy term contributes also to the width of the HF state whose intrinsic width we want to evaluate. By using the intrinsic Hamiltonian we correct for the width also. We write

$$\mathcal{H} = H - \frac{\vec{P}^2}{2mA} \qquad \text{IID(1)}$$

Here $\vec{P} = \sum_{i=1}^{A} \vec{p}_i$ is the total nuclear momentum and mA is the mass of the nucleus and $\mathcal{H}$ is the intrinsic Hamiltonian. The operator of the cm kinetic energy can be written as a

sum of one-body and two-body operators:

$$\frac{\vec{P}^2}{2mA} = \frac{1}{2m} \sum_{i=1}^{A} \vec{p}_i^{\,2} - \frac{1}{4mA} \sum_{i \neq j} (\vec{p}_i - \vec{p}_j)^2 \qquad \text{IID(2)}$$

Therefore we get

$$\mathcal{H} = \frac{1}{2} \sum_{ij} V_{ij} + \frac{1}{2} \sum_{ij} \frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} \qquad \text{IID(3)}$$

which is a pure two-body operator. Thus in actual calculations one just adds $\frac{1}{2} \sum_{ij} \frac{(p_i - p_j)^2}{2mA}$, an additional 'potential' to the two-body interaction V. With the cmm correction made, the interpretation of s.p. energies is not quite straightforward and some caution is needed. The cm energy can be taken to be the difference between the total energies with and without the cm term assuming of course that the wave function does not change much. This method for the cmm correction was used by Kerman[7] et al.

We now proceed to consider another correction to the HF wave function and energy arising from the presence of residual interactions in the HF representation. As mentioned earlier, the HF Hamiltonian is an independent particle Hamiltonian and one cannot get very far with such an approximation to the complex many-body system that a nucleus is. Residual interactions cannot be ignored and their effects on the HF energy and wave function have to be considered

in some way. One way of estimating these is via perturbation theory assuming it to be valid. In the microscopic picture the effect of residual interactions is to induce particle-hole excitations in the HF state. One advantageous feature of the HF picture is that the HF wave function is already stabilized against one particle-one hole (1ph) excitations. The second order correction, then involves only 2ph excitations. We consider this here confining ourselves only to writing down of a few relevant expressions.

The energy and the wave function corrected respectively to the 2nd order and 1st order are given by

$$E = E_{HF} + \langle \Psi_{HF} | V_{res} | \Psi_{HF} \rangle + \sum_i \frac{|\langle \Psi_{HF} | V_{res} | \Psi^i_{ph} \rangle|^2}{E_{HF} - E^{ph}_i} \qquad \text{IID(4)}$$

$$\Psi^{(1)} = \Psi_{HF} + \sum_i \frac{\langle \Psi^i_{ph} | V_{res} | \Psi_{HF} \rangle}{E_{HF} - E^{ph}_i} \Psi^i_{ph} \qquad \text{IID(5)}$$

where V_{res} is the residual interaction and Ψ^i_{ph} are the various particle-hole states built over Ψ_{HF} and E^{ph}_i their corresponding energies.

Now the 1st order term $\langle \Psi_{HF} | V_{res} | \Psi_{HF} \rangle$ in Eq. IID(4) is zero by virtue of the fact that Ψ_{HF} is a

wave function of an independent particle system. Also, the sum over the 1ph states in the third term on the r.h.s. of Eq.IID(4) vanishes. This property follows from the HF variational condition. Thus

$$\langle \Psi_{HF} | \; V_{res} | \; \Psi^{i}_{ph} \rangle \; = 0 \quad \text{for all i.}$$

Further, because V_{res} is a 2-body operator, no more than 2ph states can appear in the sum on the r.h.s. of Eq.IID(4). Therefore Eq.IID(4) reduces to

$$E = E_{HF} + \sum_{i} \frac{|\langle \Psi_{HF} | \; V_{res} | \Psi^{i}_{2ph} \rangle|^2}{E_{HF} - E^{2ph}_{i}} \qquad \text{IID(6)}$$

This can be shown to be equal to the following expression in the notation of Sec.IIB.

$$E = E_{HF} + E(2) = E_{HF} - \frac{1}{4} \sum_{\alpha\beta k\ell} \frac{\langle \alpha\beta | v | k\ell \rangle \langle k\ell | v | \alpha\beta \rangle}{\epsilon_k + \epsilon_\ell - \epsilon_\alpha - \epsilon_\beta} \qquad \text{IID(7)}$$

Here ϵ_p refers to HF s.p.energies. Now let us rewrite Eq.IID(5) as

$$\Psi^{(1)}_{HF} = \alpha \left[\Psi_{HF} + \sum_{i} C^{ph}_{i} \Psi^{i}_{ph} \right] \qquad \text{IID(8)}$$

where the factor α has been introduced so as to normalize $\Psi^{(1)}_{HF}$, i.e. $\langle \Psi^{(1)}_{HF} \; | \Psi^{(1)}_{HF} \rangle = 1$ and

$$C_i^{ph} = \frac{\langle \Psi_{ph}^i | V_{res} | \Psi_{HF} \rangle}{E_{HF} - E_i^{ph}} \qquad \text{IID(9)}$$

For reasons stated before the sum over ph states in Eq.IID(8) is only over 2ph ones. The expression for α is then

$$\alpha^2 = \frac{1}{1 + \sum_i |C_i^{2ph}|^2} \qquad \text{IID(10)}$$

Further, it can be shown that

$$\sum_i |C_i^{2ph}|^2 = \frac{1}{4} \sum_{\alpha\beta k\ell} \frac{|\langle \alpha\beta | V | k\ell \rangle|^2}{(\epsilon_\alpha + \epsilon_\beta - \epsilon_k - \epsilon_\ell)^2} \qquad \text{IID(11)}$$

E. A METHOD FOR EVALUATING THE WIDTHS OF DETERMINANTAL WAVE FUNCTIONS

Now we describe in detail a method[2] for evaluating the width defined through Eq.IIA(1). To evaluate it we make an intermediate state expansion in the complete set of orthonormal particle-hole (ph) states built on the wave function $|\Psi\rangle$. Then Eq.IIA(1) leads to

$$\sigma^2(\Psi) = \sum_{\substack{\text{all ph} \\ \text{states}}} \langle \Psi | H | \Psi_{ph} \rangle \langle \Psi_{ph} | H | \Psi \rangle - |\langle \Psi | H | \Psi \rangle|^2$$

$$= |\langle \Psi | H | \Psi_{0ph} \rangle|^2 + \sum_{1ph} |\langle \Psi | H | \Psi_{1ph} \rangle|^2$$

$$+ \sum_{2ph} |\langle \Psi | H | \Psi_{2ph} \rangle|^2 - |\langle \Psi | H | \Psi \rangle|^2$$

IIE(1)

Note that the series on the r.h.s. in Eq.IIE(1) terminates at two particle-hole states since H being a (1+2)-body operator, will not connect ph states higher than 2 ph states to the ground state. Now since $|\Psi_{0ph}\rangle \equiv |\Psi\rangle$ the first and last terms in Eq.IIE(1) are identical. Thus we get

$$\sigma^2(\Psi) = \sum_{1ph} |\langle \Psi | H | \Psi_{1ph} \rangle|^2 + \sum_{2ph} |\langle \Psi | H | \Psi_{2ph} \rangle|^2$$

IIE(2)

From Eq.IIE(2) we see that the width of the wave function $|\Psi\rangle$ arises from the one particle-hole and two particle-hole excitations only.

Since we are concerned here with the goodness of HF states, the Eq.IIE(2) can be further simplified if we remember that the first term on the right vanishes. This is because the Hamiltonian H cannot connect the HF state with the 1ph states. Thus we have

$$\sigma^2(\Psi_{HF}) = \sum_{2ph} |\langle \Psi | H | \Psi_{2ph} \rangle|^2 \qquad \text{IIE(3)}$$

We see therefore that the width of the HF ground state arises purely from the 2ph excitations.

We now give explicit expressions for the variance. In the formalism of second quantization we can write, using the notation of Sec.IIB,

$$|\Psi_{1ph}\rangle = a_k^+ a_\alpha |\Psi\rangle \qquad \text{IIE(4)}$$

and $$|\Psi_{2ph}\rangle = a_k^+ a_l^+ a_\alpha \; a_\beta |\Psi\rangle$$

Substituting from Eq.IIE(4) into Eqs.IIE(2) and IIE(3) and using Eq.IIB(3) for H we arrive at the following expressions:

$$\sigma^2(\Psi) = \sum_{\alpha k} \langle \alpha | \tilde{\epsilon} | k \rangle \langle k | \tilde{\epsilon} | \alpha \rangle + \frac{1}{4} \sum_{\alpha\beta kl} \langle \alpha\beta | v | kl \rangle \langle kl | v | \alpha\beta \rangle \qquad \text{IIE(5)}$$

and

$$\sigma^2(\Psi_{HF}) = \frac{1}{4} \sum_{\alpha\beta kl} \langle \alpha\beta | v | kl \rangle \langle kl | v | \alpha\beta \rangle \qquad \text{IIE(6)}$$

Here the matrix element $\langle\alpha|\tilde{\epsilon}|k\rangle$ of the single-particle Hamiltonian is given by

$$\langle\alpha|\tilde{\epsilon}|k\rangle = \langle\alpha|t|k\rangle + \sum_{\lambda=1}^{A}\langle\alpha\lambda|v|k\lambda\rangle \qquad \text{IIE(7)}$$

In the case of double-closed shell spherical nuclei the above expressions for σ^2 can be simplified. For these nuclei the HF s.p.states have good orbital and total angular momenta and hence when they are expanded as a finite series in the spherical jm basis states, the sum goes over radial quantum number only (see Sec.IIC). Then Eq.IIE(6) for HF variance goes over to

$$\begin{aligned}
&\sigma^2(\Psi_{HF}) \\
&= \frac{1}{4}\sum_{\{jm\tau\}_{\alpha\beta k\ell}} \sum_{\{nn'\}_{\alpha\beta k\ell}} \\
&\times\langle(nljm\tau)_\alpha,(nljm\tau)_\beta|V|(nljm\tau)_k,(nljm\tau)_\ell\rangle^* \\
&\times\langle(n'ljm\tau)_k,(n'ljm\tau)_\ell|V|(n'ljm\tau)_\alpha,(n'ljm\tau)_\beta\rangle \\
&\times C^{\alpha^*}_{n_\alpha} C^{\beta^*}_{n_\beta} C^{k^*}_{n'_k} C^{\ell^*}_{n'_\ell} C^{\alpha}_{n'_\alpha} C^{\beta}_{n'_\beta} C^{k}_{n_k} C^{\ell}_{n_\ell}
\end{aligned} \qquad \text{IIE(8)}$$

where $\sum_{\{ljm\tau\}\alpha\beta k\ell}$ means a summation over the quantum numbers l, j, m and τ of the orbits α, β, k, ℓ. Similarly for $\sum_{\{nn'\}\alpha\beta k\ell}$. It should be pointed out that five distinct types of uncoupled matrix elements of V enter into the calculation of width. These are

$$\langle pp \mid v \mid pp \rangle, \quad \langle pn \mid v \mid pn \rangle, \quad \langle p\bar{p} \mid v \mid p\bar{p} \rangle,$$

$$\langle p\bar{n} \mid v \mid p\bar{n} \rangle$$

and

$$\langle p\bar{n} \mid v \mid \bar{p}n \rangle.$$

Here p stands for a proton in a certain state and $\bar{p}$ a proton in the time reversed state. Similarly for n and $\bar{n}$. Note that of these five types only the first four enter in the ordinary Hartree-Fock calculation. Thus when width calculations are done in a large space the number of terms can easily become astronomical.

We next express the uncoupled matrix elements of V in terms of coupled two-body matrix elements V_{JT} having definite total angular momentum J and total isospin T using Clebsch-Gordan coefficients. Since V_{JT} and the expansion coefficients C are independent of m we can use the sum rules for Clebsch-Gordan coefficients and simplify the expression for σ^2. We then get

$$\sigma^2(\Psi_{HF}) = \frac{1}{4} \sum_{\substack{s_\alpha n_\alpha n'_\alpha \\ s_\beta n_\beta n'_\beta}} \sum_{\substack{s_k n_k n'_k \\ s_\ell n_\ell n'_\ell}} \sum_{JT} (2T+1)(2J+1)$$

$$\times \langle (s_\alpha n_\alpha, s_\beta n_\beta) | V | (s_k n_k, s_\ell n_\ell) \rangle_{JT}$$

$$\times \langle (s_k n'_k, s_\ell n'_\ell) | V | (s_\alpha n'_\alpha, s_\beta n'_\beta) \rangle_{JT}$$

$$\times C^{\alpha *}_{n_\alpha} C^{\beta *}_{n_\beta} C^{k *}_{n'_k} C^{\ell *}_{n'_\ell} C^{\alpha}_{n'_\alpha} C^{\beta}_{n'_\beta} C^{k}_{n_k} C^{\ell}_{n_\ell}$$

IIE(9)

F. NUMERICAL RESULTS AND DISCUSSION

We describe in this section some numerical calculations and results. As an application of the foregoing, we have carried out radial Hartree-Fock and width calculations for the double-closed shell nuclei ^{4}He, ^{16}O and ^{40}Ca. These calculations were done in the model space of first four harmonic oscillator major shells. Three different sets of effective two-body interactions were used viz. the Tabakin interaction[13], the Sussex interaction[12], and the Kuo bare interaction[11]. As is well-known each of these interactions has a claim for being "realistic", these having been derived in different ways from the two-nucleon scattering data.

The correction due to the centre of mass motion was included as described in Sec.IID. No correction arising from Coulomb repulsion has been made. Thus the binding energies presented here refer to the nuclear energies only.

First let us consider the results[4] of calculations made using the Tabakin matrix elements (Table II-1). For the oscillator length parameter b (Sec.IIC) we have used 1.81 fm for both ^{4}He and ^{16}O and 2.03 fm for ^{40}Ca. The HF energies for the Tabakin interaction are, as is well-known[7], low compared with the experimental binding energies. Further, the second-order correction in energy E(2) is approximately 20% of E_{HF} for ^{4}He and ^{16}O which is not negligible. This was first noted by Kerman et al[7]. The widths σ are large for the HF states of all the nuclei shown. In ^{16}O the HF determinant has a spread of about 24 MeV about the HF energy. This large spread implies that the ground state wave function of ^{16}O (and of other nuclei discussed) cannot be described by a single HF determinant. In fact the HF intensity shown in column 6 of the table gives us a measure of the importance of the HF state in the wave function corrected to first-order (see Eq.IID(8)).

We see from the values of α^2 (see Eq.IID(8,10)) given in Table II-1 that except for ^{4}He there is a sizable

admixture of the 2ph states in the other nuclei. In column 5, the r.m.s. radius r calculated using the HF determinant is shown. We have also studied the effect of the centre of mass motion (cmm) term on the HF potential energy as well as the width σ (HF). We find for instance in ^{16}O that the HF energy for the intrinsic Hamiltonian $\mathcal{H}$ (see Eq.IID(1)) is lower by about 11 MeV compared to that for the Hamiltonian H. The width σ (HF) is also smaller by about 2 MeV when the cmm term is included. This trend for both EHF and σ (HF) follows from the positive definite nature of the cmm term. Finally, recalling the discussion in Sec.IIA about the bounds on the exact energy we see that the interaction used here may give an additional binding of about 3 MeV per particle in ^{4}He, 1.5 MeV per particle in ^{16}O and 0.5 MeV per particle in ^{40}Ca. From Eq.IIA(3) we have

$$E - \sigma \leqslant E_o \leqslant E + \sigma$$

For the case of ^{16}O we get

$$-68.58 \leqslant E_o \leqslant -20$$

Using further the second-order correction we have

$$E_o < E_{HF} + E_2$$
$$< -53.43 \text{ MeV.}$$

We get $-68.58 \leqslant E_o < -53.43$

This tells us that if one does shell model calculation for ^{16}O with Tabakin potential (b=1.81 fm) in 4 oscillator major shells, at least one shell model eigenstate lies between -68.58 MeV and -53.43 MeV. The ground state also lies most probably in this energy interval considering the fact that E_{HF} which is a good approximation to ground state energy is -44.29 MeV.

The results of calculations with the Sussex matrix elements (b=1.7 fm) are shown in Table II-2. These results pertain to the original version of the Sussex matrix elements (Ref.12). It should be mentioned here that Elliot et al have recently published a modified version of their interaction. We see again that the widths of all three nuclei are large and that the 2p-2h correction to the HF wave function is non-negligible except for ^{4}He.

The results of our calculations using the effective interaction matrix elements of Kuo (oscillator energy parameter $\hbar\omega$= 12.5 MeV) are shown in Table II-3. This interaction gives overbinding for all the nuclei shown. Here also we find that the widths of the HF determinants of all the nuclei are large. We also see from the Tables II-2 and II-3 that the widths of the HF states resulting from Kuo's matrix elements are much bigger than those for the Sussex interaction. Also the former interaction gives larger HF

energies. Next we try to find out which interaction gives a 'better' HF solution. For this purpose we multiply the Sussex interaction by an overall factor K so that EHF (modified Sussex) = EHF (Kuo) and compare σ (modified Sussex) with σ (Kuo) (results not shown here). We find that σ (modified Sussex) is slightly smaller than σ (Kuo) and hence we may say that the two interactions are essentially equally good or bad for determining zero order (HF) wave function. The question which interactions are more suitable (in the sense of width) for carrying out HF calculations will be discussed separately in detail.

It should be remembered that both the Sussex and the Kuo matrix elements are G-matrix elements and not V-matrix elements. Thus there might be some questions raised regarding the double counting problem while evaluating widths and perturbation corrections. However, since we are calculating these quantities within the model subspace of four oscillator shells only they include unoccupied orbitals within the model space only. Furthermore, for the "bare" G-matrix elements of Kuo[11] the intermediate states tend to have high energy and therefore they would by and large lie outside the model space. Thus we may expect the double counting problem not to be very serious. Such an expectation seems to be verified "a posteriori" in view of

our results for the three interactions.

It should be emphasized again that the HF calculations of energy r.m.s. radius and the perturbation corrections to EHF and $\mathcal{V}^{(1)}$(HF) are meant basically for making comparison with the results of the new variational method (see Chap.III). These quantities have been calculated earlier and in much larger model spaces as well. Hence a detailed discussion of these quantities in the light of experimental data has not been made here. Ofcourse the evaluation of σ (HF) has not been done before in this model space of four oscillator major shells which we have used here.

G. THE EFFECT OF ENLARGING THE MODEL SPACE

The spectroscopic model space one deals with in nuclear physics is a finite vector space. In spectroscopic calculations one tries to simulate the effect of the real interaction in the infinite Hilbert space by an effective interaction in the truncated space. Several interesting problems arise from this process of reducing the infinite Hilbert space. Here we ask ourselves the question how the widths are affected by truncating or equivalently by enlarging the given finite vector space. If a wave function calculated in a given model space is transported into another larger model space and allowed to spread there, one

can then study the effect of the enlargement of space on the width of the wave function. We show in Table II-4 the results[4] of such calculations done using the three different interactions already mentioned. These calculations do not include cmm correction. To start with, we made a spherical HF calculation for ^{16}O in the space of three oscillator major shells. Then we enlarged this space by opening the full 0f-1p major shell and allowed the three-shell wave function to spread. As can be seen from Table II-4, this width is greater than both the three major shell and four major shell HF widths. All three interactions exhibit similar trends. These results show that a proper self-consistent solution in four shells (column 3) is a definite improvement over a three shell HF solution considered in the space of four shells. The difference between the two cases arises from the mixing of the 0p and 1p oscillator orbits in the HF case.

We also show in columns 5 and 6 of Table II-4 the widths for the pure oscillator determinant $(os)^4 (op)^{12}$ in the space of N=3 and N=4 oscillator shells. Again we see that the HF solutions are "better" in the sense of widths than the pure oscillator states.

Another feature we observe is that the widths become larger and larger as we enlarge the space. This would mean

that as we carry out calculations in increasingly larger spaces the HF solution gets worse; in other words there is an increasingly greater departure from the model eigenstate. We can understand this increase in width with increase in the size of the space as simply arising from the larger number of states the HF state can now mix with. It should be remembered however that although the HF state may have a sizable matrix element with a distant state the mixing of this state (in HF state) will be small because of the energy denominator which enters in the expression for the mixing amplitude.

In view of this we have evaluated[4] the ratio of the width with the spectrum span that the model nucleus has in the space. The spectrum span was determined by assuming the nuclear states (in a finite space) to have a Gaussian distribution[1] in energy. The parameters[1] which define the Gaussian density are the centroid energy (E_c) and the width. These were evaluated[1] and the ground state energy E_g determined by using Ratcliff's[1] procedure. The spectrum span was then taken to be $2(E_c - E_g)$. Although this method is probably not as accurate as some of the other methods suggested in ref.1 it provides a reasonable estimate of the spectrum span.

This ratio is shown in column 8 of Table II-4. We find that it is very small and more or less constant implying thereby that in each case the HF state can mix appreciably with only those states which lie within this small fraction of the spectrum span.

Although in our examples the widths of the states increase with an increase in the size of vector space, it might be interesting to consider interactions where the widths "saturate" as the space is enlarged. Note that since the width is a sum of squares of matrix elements, such a constraint on the interaction is non-perturbative and also more severe than demanding convergence in perturbation theory.

TABLE II-1

Some properties of the HF ground states of spherical nuclei.
Calculation in 4 oscillator major shells with centre of mass correction.
Interaction: Tabakin (b=1.81 fm for ^{4}He and ^{16}O. b=2.03 fm for ^{40}Ca).

Nucleus	EHF (MeV)	E(2) (MeV)	E(Total) (MeV)	r(HF) (fm)	α^2(HF)	Width σ(HF) (MeV)
^{4}He	-10.25	-1.93	-12.18	1.833	0.9755	12.32
^{16}O	-44.29	-9.14	-53.43	2.422	0.8620	24.29
^{40}Ca	-125.16	-15.67	-140.83	3.440	0.5587	21.34

TABLE II-2

Some properties of the HF ground states of light spherical nuclei.
Calculations in 4 oscillator major shells with centre of mass correction.
Interaction: Sussex (b=1.7 fm)

Nucleus	EHF (MeV)	E(2) (MeV)	E(Total) (MeV)	r(HF) (fm)	α^2(HF)	Width σ(HF) (MeV)
^{4}He	-12.94	-2.81	-15.75	1.817	0.9672	15.49
^{16}O	-91.84	-9.63	-101.47	2.299	0.8785	27.22
^{40}Ca	-382.99	-18.47	-401.47	2.893	0.6709	30.17

TABLE II-3

Some properties of the HF ground states of light spherical nuclei.
Calculations in 4 oscillator major shells with centre of mass correction.
Interaction: Kuo bare ($\hbar\omega$= 12.5 MeV)

Nucleus	EHF (MeV)	E(2) (MeV)	E(Total) (MeV)	r(HF) (fm)	α^2(HF)	Width σ (HF) (MeV)
^{4}He	-25.12	-5.47	-30.59	1.778	0.9439	22.61
^{16}O	-168.31	-10.08	-178.39	2.242	0.8932	30.34
^{40}Ca	-550.89	-30.24	-581.13	3.047	0.5799	38.62

TABLE II-4

Effect of enlargement of space on width (σ)
Nucleus: ^{16}O
N is the number of oscillator major shells in which σ was calculated

Interaction	$\sigma(\Psi^{N}_{HF})$		$\sigma(\Psi^{N=3}_{HF}$ in 4 major shell space)	$\sigma(\Psi^{N}_{pure}$ H.O.)		Spectrum span S		Ratio $\sigma(\Psi^{N}_{HF})/S$	
	N=3	N=4		N=3	N=4	N=3	N=4	N=3	N=4
Sussex (b=1.7fm)	29.91	29.56	33.39	29.29	34.43	536.18	782.28	0.0390	0.0378
Kuo ($\hbar\omega$=12.5 MeV)	26.24	32.71	48.47	29.74	49.77	541.42	790.24	0.0485	0.0414
Tabakin (b=1.81fm)	18.29	26.49	29.99	19.41	30.73	461.44	672.03	0.0396	0.0394

REFERENCES FOR CHAPTER II

1. J.B. French and K.F. Ratcliff, Phys. Rev. C3, 94 (1971); K.F. Ratcliff, ibid, 3, 117 (1971).
2. J.C. Parikh and J.P. Svenne, Phys. Rev.C6, 34 (1972).
3. V. Satyan and J.C. Parikh, in Proc.Nucl.Phys. and Solid State Physics Symposium, Chandigarh (1973), 15B, 289;
   V. Satyan and J.C. Parikh, in Proc.Int.Conf.on Nuclear Physics, Munich (1973), Vol.1, p.52.
4. V. Satyan and J.C. Parikh, Physical Review C(to appear).
5. I. Kelson and G. Shadmon, Ann.of Phys.63, 497 (1971).
6. N. Ullah and R.K. Nesbet, Nucl.Phys. 39, 239 (1962); Phys. Rev. 134B, 308 (1964).
7. A.K. Kerman, J.P. Svenne, F.M.H. Villars, Phys. Rev. 147, 710 (1966).
8. G. Ripka, Advances in Nuclear Physics, edited by M. Baranger and E.Vogt (Plenum Press, New York, 1968), Vol1, Chap.3.
9. R.M. Tarbutton and K.T.R. Davies, Nucl. Phys. A120, 1 (1968).
10. J.W. Negele, Phys. Rev.C1, 1260 (1970).
11. T.T.S. Kuo, Nucl.Phys.A103, 71 (1967).

12. J.P. Elliot et al, Nucl. Phys. A121, 241 (1968).

13. F. Tabakin, Ann. of Phys. 30, 51 (1964);
D.M. Clement and E.U. Baranger, Nucl. Phys. A108, 27 (1968).

CHAPTER III

A VARIATIONAL METHOD BASED ON MINIMIZATION OF ENERGY VARIANCE

A. INTRODUCTION

We have so far discussed the concept of width of a wave function and applied this concept to the study of goodness of some HF determinantal wave functions. We discussed in chapter II two different criteria for the goodness of wave functions and pointed out that corresponding to each criterion one can set up a variational procedure for obtaining approximate wave functions. It was also pointed out that if we allowed for the most general variation in the wave function then each of these procedures would be equivalent to solving the Schroedinger equation. We obtain different variational solutions only when we put restrictions on the variational wave functions. For determinantal states, the energy minimization leads to the well-known Hartree-Fock procedure. This we have discussed briefly in the previous chapter. Our results of the calculations described therein showed that the widths of HF states of double-closed shell nuclei are large. That is to say, these HF states are far from being the ground state eigenfunction of the model Hamiltonian although they are

the 'best' determinants in the sense of their energies being minimum. The question then arises whether a single Slater determinant which has minimum energy variance instead of minimum energy provides a better description of the ground state of the nucleus[1,2]. We take up this question in this chapter and study it in great detail. First we develop this alternative variational procedure and then apply it to double-closed shell nuclei whose HF wave functions and widths we have already obtained as discussed in chapter II. Finally, we make a comparative study of the two distinct variational procedures viz. the HF procedure and the variance minimization procedure.

B. FORMULATION OF THE METHOD

Consider a Slater determinant $|\Psi\rangle$ (see Eq.IIB(1)) as an approximation to an eigenstate of a nucleus consisting of A nucleons. To determine $|\Psi\rangle$ let us require that its energy variance $\sigma^2(\Psi)$ as defined in Eq.IIA(1) be stationary when $|\Psi\rangle$ is varied. This means

$$\delta \frac{\sigma^2(\Psi)}{\langle\Psi|\Psi\rangle} = \delta \frac{\langle\Psi|H^2|\Psi\rangle - |\langle\Psi|H|\Psi\rangle|^2}{\langle\Psi|\Psi\rangle} = 0. \qquad \text{IIIB(1)}$$

Here δ denotes the most general variation of $|\Psi\rangle$. If we require further that $|\Psi\rangle$ should be normalized then the variations in $|\Psi\rangle$ will be restricted to first order variations only. We can then write Eq.III$_B$(1) as

$$\delta\left[\langle\Psi|H^2|\Psi\rangle - |\langle\Psi|H|\Psi\rangle|^2\right] = 0. \qquad \text{IIIB(2)}$$

Since $|\Psi\rangle$ and its conjugate $\langle\Psi|$ can be varied independently we choose to vary $\langle\Psi|$. Now for a first order change $\delta\langle\Psi|$ in $\langle\Psi|$ we must have

$$\delta\langle\Psi| = \eta\langle\Psi_{1ph}| \qquad \text{IIIB(3)}$$

where η is an infinitesimal and $\langle\Psi_{1ph}|$ is a one particle-one hole state built on $\langle\Psi|$. With this the Eq.IIIB(2) becomes

$$\langle\delta\Psi|H^2|\Psi\rangle - 2\langle\Psi|H|\Psi\rangle\langle\delta\Psi|H|\Psi\rangle = 0.$$

IIIB(4)

i.e.

$$\langle\Psi_{1ph}|H^2|\Psi\rangle - 2\langle\Psi|H|\Psi\rangle\langle\Psi_{1ph}|H|\Psi\rangle = 0.$$

IIIB(5)

In order to evaluate the first term in Eq.IIIB(5) we carry out an intermediate state expansion where we choose for the intermediate states the complete set of particle-hole (ph) states $\{\Psi'_{nph}\}$ (n=0,1,2...) built on the state $|\Psi\rangle$. Then Eq.IIIB(5) gives

$$\langle\Psi_{1ph}|H|\Psi'_{0ph}\rangle\langle\Psi'_{0ph}|H|\Psi\rangle + \sum_{\Psi'_{1ph}}\langle\Psi_{1ph}|H|\Psi'_{1ph}\rangle\langle\Psi'_{1ph}|H|\Psi\rangle + \sum_{\Psi'_{2ph}}\langle\Psi_{1ph}|H|\Psi'_{2ph}\rangle\langle\Psi'_{2ph}|H|\Psi\rangle - 2\langle\Psi|H|\Psi\rangle\langle\Psi_{1ph}|H|\Psi\rangle = 0. \qquad \text{IIIB(6)}$$

In Eq.IIIB(6) terms of the type $\langle\Psi_{1ph}|H|\Psi'_{nph}\rangle \times \langle\Psi'_{nph}|H|\Psi\rangle$ where n=3,4... do not contribute. This is due to the fact that the Hamiltonian H being a (1+2)-body operator can connect at most a two particle-hole state to the state Ψ. Further, since $|\Psi'_{0ph}\rangle \equiv |\Psi\rangle$, Eq.IIIB(6) simplifies to

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$$\langle \Psi_{1ph}|H|\Psi'_{0ph}\rangle\langle\Psi'_{0ph}|H|\Psi\rangle + \sum_{\Psi'_{1ph}} \langle \Psi_{1ph}|H|\Psi'_{1ph}\rangle\langle\Psi'_{1ph}|H|\Psi\rangle + \sum_{\Psi'_{2ph}} \langle \Psi_{1ph}|H|\Psi'_{2ph}\rangle\langle\Psi'_{2ph}|H|\Psi\rangle - 2\langle\Psi|H|\Psi\rangle\langle\Psi_{1ph}|H|\Psi\rangle = 0. \qquad \text{IIIB(6)}$$

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$$\sum_{\Psi'_{1ph}} \langle \Psi_{1ph} | H | \Psi'_{1ph} \rangle \langle \Psi'_{1ph} | H | \Psi \rangle$$
$$+ \sum_{\Psi'_{2ph}} \langle \Psi_{2ph} | H | \Psi'_{2ph} \rangle \langle \Psi'_{2ph} | H | \Psi \rangle$$
$$- \langle \Psi | H | \Psi \rangle \langle \Psi_{1ph} | H | \Psi \rangle = 0.$$

IIIB(7)

Next we briefly describe the evaluation of various terms in Eq.IIIB(7). We adopt the notation described in sec.IIB. Consider a term $\langle \Psi_{1ph} | H | \Psi'_{1ph} \rangle \langle \Psi'_{1ph} | H | \Psi \rangle$ in the sum over $|\Psi'_{1ph}\rangle$ states in Eq.IIIB(7). In the second quantization formalism this becomes

$$\langle \Psi | a^+_\alpha a_k H a^+_l a_\beta | \Psi \rangle \langle \Psi | a^+_\beta a_l H | \Psi \rangle \qquad \begin{matrix} \alpha, \beta, \text{occupied} \\ k, l, \text{unoccupied} \end{matrix}$$

IIIB(8)

where we have written $\langle \Psi_{1ph} | = \langle \Psi | a^+_\alpha a_k$ and $|\Psi'_{1ph}\rangle = a^+_l a_\beta | \Psi \rangle$. Substituting for H from Eq.IIB(3) we get

$$\langle\Psi|a_\alpha^+ a_k H a_l^+ a_\beta|\Psi\rangle$$

$$= \sum_{pq}\langle p|t|q\rangle\langle\Psi|a_\alpha^+ a_k a_p^+ a_q a_l^+ a_\beta|\Psi\rangle$$

$$+ \frac{1}{4}\sum_{\substack{pq\\p'q'}}\langle pq|V|p'q'\rangle\langle\Psi|a_\alpha^+ a_k a_p^+ a_q^+ a_{q'} a_{p'} a_l^+ a_\beta|\Psi\rangle$$

IIIB(9)

Now we can apply Wick's Theorem to the products of operators here and simplify. On carrying out the contractions and the sums we get

$$\sum_{\Psi'_{iph}}\langle\Psi_{iph}|H|\Psi'_{iph}\rangle\langle\Psi'_{iph}|H|\Psi\rangle$$

$$= \langle\Psi|H|\Psi\rangle\langle k|\tilde{\epsilon}|\alpha\rangle + \sum_\ell\langle k|\tilde{\epsilon}|\ell\rangle\langle\ell|\tilde{\epsilon}|\alpha\rangle$$

$$-\sum_\beta\langle k|\tilde{\epsilon}|\beta\rangle\langle\beta|\tilde{\epsilon}|\alpha\rangle - \sum_{\beta\ell}\langle\ell|\tilde{\epsilon}|\beta\rangle\langle\beta k|V|\alpha\ell\rangle$$

IIIB(10)

Here $\langle p|\tilde{\epsilon}|q\rangle$ is a matrix element of the one-body Hamiltonian defined as follows:

$$\langle p|\tilde{\epsilon}|q\rangle = \langle p|t|q\rangle + \sum_{\lambda\ \text{occupied}}\langle p\lambda|v|q\lambda\rangle$$

IIIB(11)

To evaluate the terms in the sum over $|\Psi'_{2ph}\rangle$ states we write

$$\langle\Psi_{1ph}| = \langle\Psi| a^+_\alpha a_k$$

$$|\Psi'_{2ph}\rangle = a^+_l a^+_m a_\beta a_\gamma |\Psi\rangle$$

Then

$$\langle\Psi_{1ph}| H |\Psi'_{2ph}\rangle\langle\Psi'_{2ph}| H |\Psi\rangle$$

$$= \langle\Psi| a^+_\alpha a_k H a^+_l a^+_m a_\beta a_\gamma |\Psi\rangle\langle\Psi| a^+_\gamma a^+_\beta a_m a_l H |\Psi\rangle$$

IIIB(12)

We next proceed to evaluate the various terms using Wick's Theorem and finally arrive at the following expression

$$\sum_{\Psi'_{2ph}} \langle\Psi_{1ph}|H|\Psi'_{2ph}\rangle\langle\Psi'_{2ph}|H|\Psi\rangle$$

$$= \sum_{\beta l} \langle\beta|\tilde{\epsilon}|l\rangle\langle kl|V|\alpha\beta\rangle$$

$$+ \tfrac{1}{2} \sum_{\beta lm} \langle\beta k|V|lm\rangle\langle lm|V|\beta\alpha\rangle$$

$$- \tfrac{1}{2} \sum_{\beta\gamma m} \langle km|V|\beta\gamma\rangle\langle\beta\gamma|V|\alpha m\rangle$$

IIIB(13)

Now the last term in Eq.IIIB(7) is just $\langle\Psi|H|\Psi\rangle\langle k|\tilde{\epsilon}|\alpha\rangle$ which cancels exactly the first term in Eq.IIIB(10). Substituting for the various terms in Eq.IIIB(7) from Eqs.IIIB(10) and IIIB(13) we finally obtain the following equation

$$\sum_{\ell}\langle k|\tilde{\epsilon}|\ell\rangle\langle\ell|\tilde{\epsilon}|\alpha\rangle - \sum_{\beta}\langle k|\tilde{\epsilon}|\beta\rangle\langle\beta|\tilde{\epsilon}|\alpha\rangle$$

$$+\sum_{\beta\ell}\langle\ell|\tilde{\epsilon}|\beta\rangle\langle\beta k|V|\ell\alpha\rangle + \sum_{\beta\ell}\langle\beta|\tilde{\epsilon}|\ell\rangle\langle k\ell|V|\alpha\beta\rangle$$

$$+\frac{1}{2}\sum_{\beta\ell m}\langle\beta k|V|\ell m\rangle\langle\ell m|V|\beta\alpha\rangle$$

$$-\frac{1}{2}\sum_{\beta\gamma m}\langle km|V|\beta\gamma\rangle\langle\beta\gamma|V|\alpha m\rangle$$

$$=0. \qquad \text{IIIB(14)}$$

It should be recalled that Greek letters $\alpha, \beta, \gamma, \lambda$, etc. refer to occupied s.p.states and k,l,m, etc. to the unoccupied s.p.states.

Next we define a single-particle operator

$$\hat{\sigma}^2 = \sum_{pq}\Big\{\sum_{\ell}\langle p|\tilde{\epsilon}|\ell\rangle\langle\ell|\tilde{\epsilon}|q\rangle$$

$$-\sum_{\beta}\langle p|\tilde{\epsilon}|\beta\rangle\langle\beta|\tilde{\epsilon}|q\rangle$$

$$+\sum_{\beta\ell}\langle\ell|\tilde{\epsilon}|\beta\rangle\langle\beta p|v|\ell q\rangle+\sum_{\beta\ell}\langle\beta|\tilde{\epsilon}|\ell\rangle\langle p\ell|v|q\beta\rangle$$

$$+\frac{1}{2}\sum_{\beta\ell m}\langle\beta p|v|\ell m\rangle\langle\ell m|v|\beta q\rangle$$

$$-\frac{1}{2}\sum_{\beta\gamma m}\langle pm|v|\beta\gamma\rangle\langle\beta\gamma|v|qm\rangle\Big\}a_p^+ a_q \qquad \text{IIIB(15)}$$

where p,q denote arbitrary single particle states. Then from Eq.IIIB(14) we have

$$\langle k|\hat{\sigma}^2|\alpha\rangle = 0 \qquad \alpha \leq A,\ k > A \qquad \text{IIIB(16)}$$

Eq.IIIB(16) tells us that the single-particle operator $\hat{\sigma}^2$ does not connect the occupied single particle states to the unoccupied ones. This property of $\hat{\sigma}^2$ allows us to diagonalize $\hat{\sigma}^2$ in the space of occupied s.p.states only to obtain its eigenvalues and eigenfunctions. We can then write

$$\hat{\sigma}^2|\lambda\rangle = W_\lambda|\lambda\rangle \qquad \text{IIIB(17)}$$

where λ now label the occupied s.p.states and W_λ are the eigenvalues of $\hat{\sigma}^2$. Eq.IIIB(17) is apparently the eigenvalue equation for the operator $\hat{\sigma}^2$. This may be

compared with its HF analogue (Eq.IIB(10)). We see from Eq.IIIB(15) that $\hat{\sigma}^2$ is a functional of occupied s.p. wave functions. Therefore Eq.IIIB(17) has to be solved in a self-consistent way. The procedure here is the same as in HF (see Sec.IIB) and consists in setting up an iterative cycle by starting off with a trial set of s.p. wave functions. Using this trial set one calculates the $\hat{\sigma}^2$ matrix and diagonalizes it to produce a new set of trial wave functions for the next iteration . This cycle is stopped when the incoming and the outgoing s.p. wave functions are the same i.e. the s.p. wave functions are self-consistent. With these wave functions one computes the variance of the determinantal wave function using the Eq.IIE(5). This then is the determinantal wave function having minimum variance.

Once the minimum variance wave function Ψ_σ has been obtained, evaluation of physical quantities like energy (Eq.IIB(14)), r.m.s. radius (Eq.IIC(8)) etc. is straightforward.

C. PERTURBATION THEORY CORRECTIONS

Although the minimum variance wave function has built into it some particle-hole correlations it is nevertheless an approximate wave function. Hence it is necessary

to evaluate the corrections to it arising from the presence of residual interactions. It was mentioned in Sec.IID that a proper way to take care of the effects of the residual interactions is to treat them in perturbation theory. For the HF state the first nonvanishing correction comes from the second order terms these consisting of 1ph and 2ph excitations to the HF state. Further, the 1ph terms vanish by virtue of the HF minimal condition. Thus the second order correction to the HF consists solely of 2ph corrections. This simplification obtaining in the HF picture is unfortunately not available in the present method. In other words, the zeroth order wave function Ψ_0 has non-vanishing matrix elements with both 1ph and 2ph states. This will be clear if we consider the minimal condition for energy variance viz.

$$\langle \delta\Psi | (H - \langle \Psi | H | \Psi \rangle)^2 | \Psi \rangle = 0 \qquad \text{IIIC(1)}$$

from which it does not follow that

$$\langle \delta\Psi | H | \Psi \rangle = 0 \qquad \text{IIIC(2)}$$

which is the condition required for the vanishing of 1ph correlations to Ψ .

Now we give the explicit forms for system energy and wave function correct upto second and first order respectively. In the notation of Sec.IIB we get

$$E = \langle \Psi_\sigma | H | \Psi_\sigma \rangle + \sum_{1ph} \frac{|\langle \Psi_\sigma | H | \Psi_{1ph} \rangle|^2}{E_\sigma - E_{1ph}} + \sum_{2ph} \frac{|\langle \Psi_\sigma | H | \Psi_{2ph} \rangle|^2}{E_\sigma - E_{2ph}}$$

$$= E_\sigma + \sum_{\alpha k} \frac{|\langle \alpha | \tilde{\epsilon} | k \rangle|^2}{\epsilon_\alpha - \epsilon_k} + \frac{1}{4} \sum_{\alpha\beta k\ell} \frac{|\langle \alpha\beta | v | k\ell \rangle|^2}{\epsilon_\alpha + \epsilon_\beta - \epsilon_k - \epsilon_\ell}$$

IIIC(3)

and

$$\Psi_\sigma^{(1)} = \Psi_\sigma + \sum_{1ph} \frac{\langle \Psi_\sigma | H | \Psi_{1ph} \rangle}{E_\sigma - E_{1ph}} \Psi_{1ph} + \sum_{2ph} \frac{\langle \Psi_\sigma | H | \Psi_{2ph} \rangle}{E_\sigma - E_{2ph}} \Psi_{2ph}$$

$$= \Psi_\sigma + \sum_{\alpha k} \frac{\langle \alpha | \tilde{\epsilon} | k \rangle}{\epsilon_\alpha - \epsilon_k} \Psi_{1ph}^{\alpha k} + \frac{1}{4} \sum_{\alpha\beta k\ell} \frac{\langle \alpha\beta | v | k\ell \rangle}{\epsilon_\alpha + \epsilon_\beta - \epsilon_k - \epsilon_\ell} \Psi_{2ph}^{\alpha\beta k\ell}$$

IIIC(4)

In Eqs.IIIC(3) and IIIC(4) Ψ_{1ph}, Ψ_{2ph} are particle-hole states built on Ψ_σ and E_σ, E_{1ph} and E_{2ph} are the expectation values of the Hamiltonian H taken with

Ψ_σ, Ψ_{1ph} and Ψ_{2ph} respectively. α, β, k, ℓ, are the s.p. states in Ψ_σ and ϵ_α etc. are the expectation values of the one-body operator $\tilde{\epsilon}$ evaluated in states α, etc. For the definition of $\tilde{\epsilon}$ see Eq.IIIB(11). To normalize $\Psi_\sigma^{(1)}$ we write

$$\Psi_\sigma^{(1)} = \alpha\left[\Psi_\sigma + \sum_{1ph} C_{1ph}\,\Psi_{1ph} + \sum_{2ph} C_{2ph}\,\Psi_{2ph}\right]$$

IIIC(5)

where α is the normalization factor and the C's are the expansion coefficients. Using $\langle \Psi_\sigma^{(1)} | \Psi_\sigma^{(1)} \rangle = 1$ we get

$$\alpha^2 = \left[1 + \sum_{\alpha k} \frac{|\langle \alpha|\tilde{\epsilon}|k\rangle|^2}{\epsilon_\alpha - \epsilon_k} + \frac{1}{4}\sum_{\alpha\beta k\ell} \frac{|\langle \alpha\beta|V|k\ell\rangle|^2}{\epsilon_\alpha + \epsilon_\beta - \epsilon_k - \epsilon_\ell}\right]^{-1}$$

IIIC(6)

D. NUMERICAL RESULTS AND COMPARISON WITH THE HF METHOD

We consider in this section the application of the variational method described in Sec.IIIB to some double-closed shell nuclei[1,2]. These nuclei are not deformed in their ground states and hence a good approximation to them would be Slater determinants which are spherically symmetric.

$$\langle s_\alpha n_\alpha | \hat{\sigma}^2 | s_\alpha n'_\alpha \rangle$$

$$= \sum_{s_\ell n_\ell n'_\ell} \langle s_\alpha n_\alpha | \tilde{\epsilon} | s_\ell n_\ell \rangle \langle s_\ell n'_\ell | \tilde{\epsilon} | s_\alpha n'_\alpha \rangle \hat{\delta}_{\alpha\ell} C^{\ell *}_{n'_\ell} C^{\ell}_{n_\ell}$$

$$- \sum_{s_\beta n_\beta n'_\beta} \langle s_\alpha n_\alpha | \tilde{\epsilon} | s_\beta n_\beta \rangle \langle s_\beta n'_\beta | \tilde{\epsilon} | s_\alpha n'_\alpha \rangle \hat{\delta}_{\alpha\beta} C^{\beta *}_{n'_\beta} C^{\beta}_{n_\beta}$$

$$+ \frac{1}{2(2J_\alpha+1)} \sum_{\substack{s_\beta n_\beta n'_\beta \\ s_\ell n_\ell n'_\ell}} \Bigg[\langle s_\ell n_\ell | \tilde{\epsilon} | s_\beta n_\beta \rangle \hat{\delta}_{\alpha\beta} \sum_{JT} (2T+1)(2J+1) \times$$

$$\langle (s_\beta n'_\beta, s_\alpha n_\alpha) | V | (s_\ell n'_\ell, s_\alpha n'_\alpha) \rangle_{JT} C^{\ell *}_{n_\ell} C^{\beta *}_{n'_\beta} C^{\ell}_{n'_\ell} C^{\beta}_{n_\beta}$$

$$+ \langle s_\beta n_\beta | \tilde{\epsilon} | s_\ell n_\ell \rangle \hat{\delta}_{\alpha\beta} \sum_{JT} (2T+1)(2J+1) \times$$

$$\langle (s_\ell n'_\ell, s_\alpha n_\alpha) | V | (s_\beta n'_\beta, s_\alpha n'_\alpha) \rangle_{JT} C^{\beta *}_{n_\beta} C^{\ell *}_{n'_\ell} C^{\beta}_{n'_\beta} C^{\ell}_{n_\ell} \Bigg]$$

$$+ \frac{1}{2(2J_\alpha+1)} \cdot \frac{1}{2} \sum_{\substack{s_\beta n_\beta n'_\beta \\ s_\ell n_\ell n'_\ell \\ s_m n_m n'_m}} \sum_{JT} (2T+1)(2J+1) \langle (s_\beta n_\beta, s_\alpha n_\alpha) | V | (s_\ell n_\ell, s_m n_m) \rangle_{JT} \times$$

$$\times \langle (s_\ell n'_\ell, s_m n'_m) | V | (s_\beta n'_\beta, s_\alpha n'_\alpha) \rangle_{JT} C^{\beta *}_{n_\beta} C^{\ell *}_{n'_\ell} C^{m *}_{n'_m} C^{\beta}_{n'_\beta} C^{\ell}_{n_\ell} C^{m}_{n_m}$$

$$- \frac{1}{2(2J_\alpha+1)} \cdot \frac{1}{2} \sum_{\substack{s_\beta n_\beta n'_\beta \\ s_r n_r n'_r \\ s_m n_m n'_m}} \sum_{JT} (2T+1)(2J+1) \langle (s_\alpha n_\alpha, s_m n_m) | V | (s_\beta n_\beta, s_r n_r) \rangle_{JT} \times$$

$$\times \langle (s_\beta n'_\beta, s_r n'_r) | V | (s_\alpha n'_\alpha, s_m n'_m) \rangle_{JT} C^{\beta *}_{n'_\beta} C^{\gamma *}_{n'_\gamma} C^{m *}_{n_m} C^{\beta}_{n_\beta} C^{\gamma}_{n_\gamma} C^{m}_{n'_m}$$

The assumption of spherical symmetry reflects itself in the spherical symmetry of the s.p. wave functions. Thus the admixture is only in the radial part of the s.p. wave functions. We have already discussed these points in connection with radial HF (Sec.IIC). We give in Eq.IIID(1) expression for the matrix elements of the one-body operator $\hat{\sigma}^2$ (Eq.IIIB(15)) in the harmonic oscillator orbitals $|nlj\rangle$ using the notation of Sec.IIB. The delta function in Eq.IIID(1) has the same definition as the one used in Eq.IIC(4). The $C^{\beta}_{n_\beta}$ etc. are the expansion coefficients (see Eq.IIC(3)).

The high degree of non-linearity of the set of equations in IIID(1) is evident. Whereas the Hartree-Fock method gives rise to a set of simultaneous cubic equations in C's (see Eq.IIB(12)) the present method yields a set of simultaneous equations of the seventh degree in C's. Consequently the numerical solution of Eq.IIID(1) becomes harder and poses some convergency problems. Another source of complication is the existence of multiple minima. We have not studied all the solutions corresponding to different local minima, but they may provide some interesting information about high lying states having J=0 and T=0. For comparison with the HF results we have always chosen the

solution having the lowest energy. We present in Fig.1 a plot of the variation of σ^2 for ^{16}O with determinantal wave function Ψ . This is a calculation in the first three harmonic oscillator major shells and therefore there is only one variational parameter viz. $C(os_{\frac{1}{2}})$. This calculation was done with Tabakin (b=1.81 fm) force with centre of mass correction included. It is seen from this plot that σ^2 goes to a minimum in the neighbourhood of the HF minimum. Further, we also see another minimum of σ^2 coming at a high energy. We also present in Fig.2 a plot of the expectation values $|\langle\Psi|H|\Psi\rangle|^2$ and $\langle\Psi|H^2|\Psi\rangle$ for ^{16}O against the parameter $C(os_{\frac{1}{2}})$. This is also a three shell calculation with Tabakin (b=1.81 fm) matrix elements with cmm correction. It is evident that the two quantities vary in a similar fashion with variation in $C(os_{\frac{1}{2}})$. An interesting feature of this plot is that $\langle\Psi|H^2|\Psi\rangle$ also has a minimum near the HF energy minimum. It might be interesting to investigate whether this feature extends also to the higher powers of H i.e. whether the expectation values $\langle\Psi|H^p|\Psi\rangle$ $(p>2)$ where Ψ is a Slater determinant, also become minimum near the HF minimum. All these are aspects which remain to be studied further.

Fig.1

Variation of $\sigma^2(\Psi)$ with determinantal wave function Ψ. The nucleus is ^{16}O in the first three harmonic oscillator major shells. Thus there is only one variational parameter in Ψ viz., $C(nlj)=C(os_{\frac{1}{2}})$ which is the amplitude of the $|os_{\frac{1}{2}}\rangle$ state in the orbit $|s_{\frac{1}{2}}\rangle$. The two-body interaction used here is Tabakin force (b=1.81 fm). Y-axis shows σ^2 in powers of ten (units MeV^2).

Fig.2

Variation of the expectation values $|\langle\Psi|H|\Psi\rangle|^2$ and $\langle\Psi|H^2|\Psi\rangle$ with determinantal wave function Ψ. The variational parameter is $C(os_{\frac{1}{2}})$. This plot is for ^{16}O in three major shells with Tabakin interaction (b=1.81 fm). Y-axis shows the two quantities in powers of ten (units MeV^2).

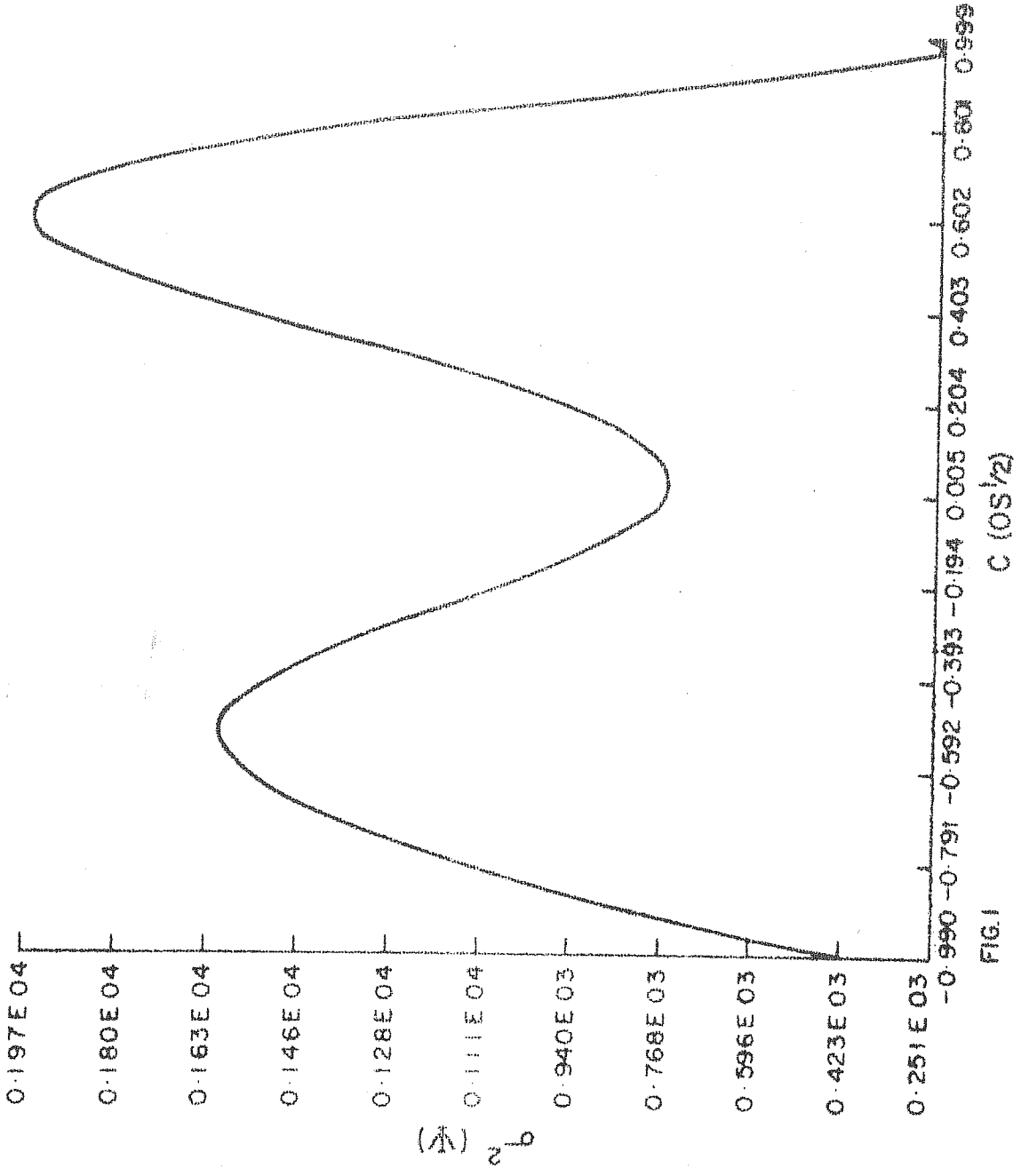

0·197E04
0·180E04
0·163E04
0·146E04
0·128E04
0·111E04
0·940E03
0·768E03
0·596E03
0·423E03
0·251E03
q^{-2} (Å)
-0·990 -0·791 -0·592 -0·393 -0·194 0·005 0·204 0·403 0·602 0·801 0·999
C (OS½)

FIG. 1

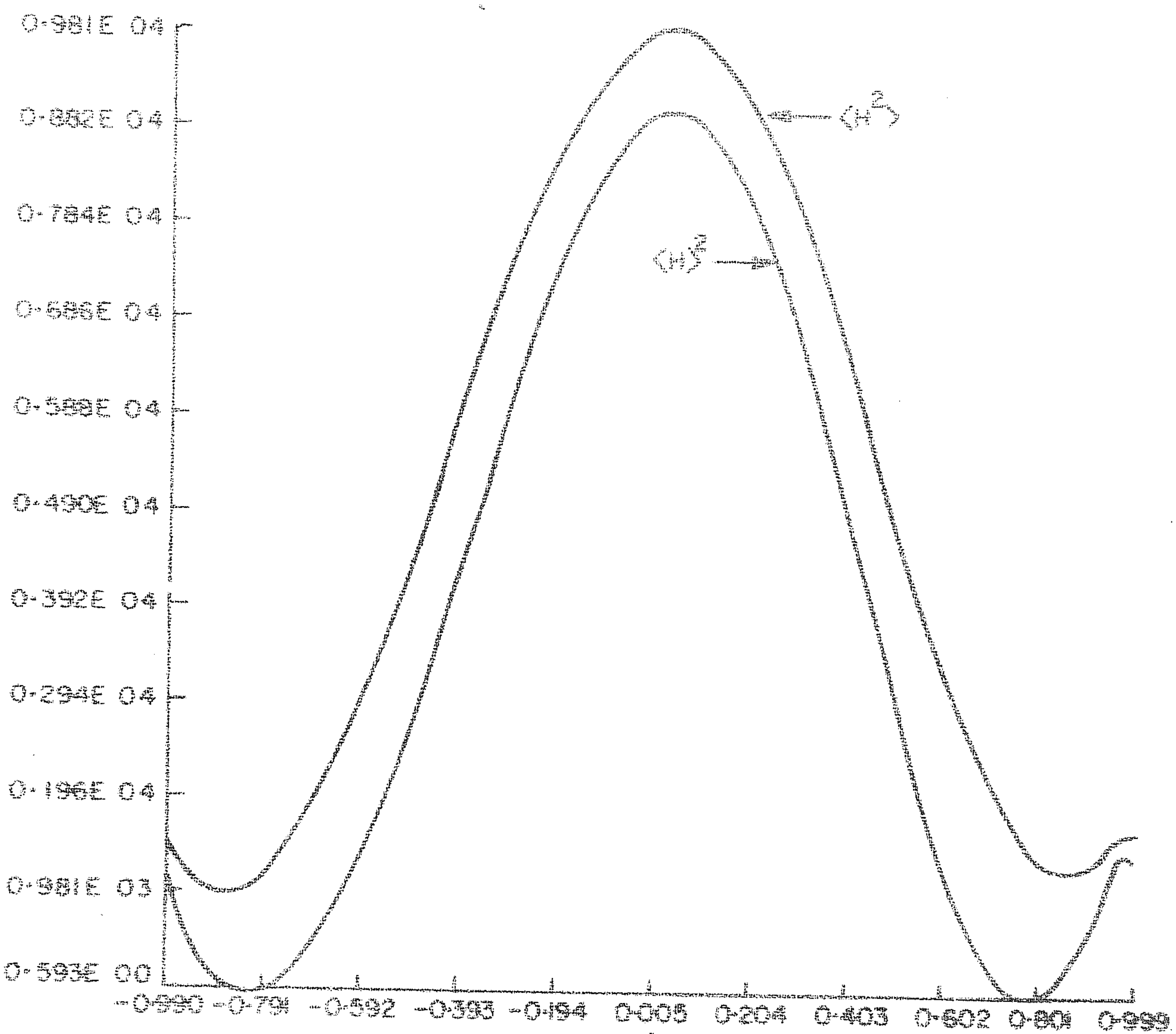

0·981E 04
0·882E 04
0·784E 04
0·686E 04
0·588E 04
0·490E 04
0·392E 04
0·294E 04
0·196E 04
0·981E 03
0·593E 00
-0·990
-0·791
-0·592
-0·393
-0·194
0·005
0·204
0·403
0·602
0·801
0·999
$\langle H^2 \rangle$
$\langle H \rangle^2$
C (OS ½)

FIG. 2

We now consider the energy variance minimization calculations which we have carried out for the double-closed shell nuclei ^{4}He, ^{16}O and ^{40}Ca. These calculations were done in the model space of first four oscillator major shells. The three different sets of effective two-body interactions discussed in Chapter II were used here also viz. the Tabakin interaction, the Sussex interaction and the Kuo bare interaction. We have included in these calculations correction due to the centre of mass motion. The procedure for doing this has already been discussed in Sec. IID. Coulomb corrections, however, have not been included in these calculations.

We show in Tables III-1, III-2 and III-3 the results[1,2] of calculations made with Tabakin (b=1.81 and 2.03 fm), Sussex (b=1.7 fm) and Kuo ($\hbar\omega$=12.5 MeV) matrix elements respectively. In these Tables we show the same quantities as were shown in Tables II-1, II-2 and II-3 for the HF solution (see Chapter II). We see that the energies obtained by the two different variational procedures (the HF and the variance methods) are nearly equal in all the nuclei studied. This shows that a variance minimum solution exists in the neighbourhood of the HF solution. The maximum difference in the energies of about 2.3 MeV for Tabakin, 2.1 MeV for Sussex and 1.9 MeV for Kuo interactions obtained

by the two procedures is found in the case of ^{16}O. Further, the minimum variance obtained is at best only a few per cent smaller than the variance of the HF solution. This means that the wave function obtained by minimization of σ^2 is not really very different from the HF one in so far as these studies indicate. In other words, the HF solution nearly minimizes the width in the ground state domain.

We have also calculated using the minimum variance wave function, second-order perturbation corrections to the energy arising from 1ph and 2ph excitations (see Sec. IIIC). The total correction in energy is denoted by E(2) in Tables III-1, III-2 and III-3. It should be emphasized that unlike the HF solution the state Ψ_σ gives non-zero contribution from 1ph intermediate states.

It is seen that the second-order perturbation corrections E(2) obtained for the two solutions do not differ very much . However, the 2ph intermediate state contribution to E(2) calculated for the minimum variance wave function is found to be less than that obtained for the HF wave functions (these results are not shown here). The reason for this is as follows: in minimizing energy variance we are minimizing the sum of one particle-hole and two particle-hole contributions to the ground state wave function as is

clear from Eq.IIE(2). Thus the minimum variance wave function already contains some two particle-hole contributions in contrast to the HF wave function which does not and cannot contain such a contribution. We find that in the case of ^{16}O this difference in the 2ph second-order correction is about 1.7 MeV for all the three interactions used. Thus the present method provides us with a determinantal wave function that has less 2ph second order perturbation correction than the HF determinant. Let us next consider the intensity of the state Ψ_σ in the wave function $\Psi_\sigma^{(1)}$ (corrected to first order in perturbation theory). If we compare the numbers in column 6 of Tables II-1 and III-3, Tables II-2 and III-2, and Tables II-3 and III-3, we find that in almost every case the intensity of Ψ_σ in $\Psi_\sigma^{(1)}$ is almost the same as the intensity of Ψ_{HF} in $\Psi_{HF}^{(1)}$.

We show in column 5 in Tables III-1, III-2 and III-3 the r.m.s. mass radius r obtained by using Ψ_σ. It is seen that the minimum variance method gives a smaller nuclear radius than the HF method.

In Tables III-4, III-5 and III-6, we show the single particle energies for the interactions of Tabakin, Sussex and Kuo respectively. It is seen from these results that the present variational method generates a single-particle

potential well that is much deeper compared to the HF potential well. In the case of ^{16}O, the lowest occupied level ($s_{\frac{1}{2}}$) in Ψ_σ is about 2-3 MeV (considering all three interactions) below its HF counterpart. Now if we consider the total potential energy of Ψ_σ, it is found to be larger than Ψ_{HF}. But we find that the total kinetic energy of Ψ_σ is also larger than Ψ_{HF} and the net result is that the total energy of Ψ_σ is smaller than Ψ_{HF}.

Next, it is seen that this variational method gives rise to larger spin-orbit splittings as compared with the HF method. For example, in the case of ^{16}O calculation with Tabakin matrix elements the lowest $p_{3/2} - p_{1/2}$ splitting in Ψ_σ is larger by 1.5 MeV than its splitting in Ψ_{HF}; and the $d_{5/2} - d_{3/2}$ splitting in Ψ_σ is larger by about 0.83 MeV. The differences in spin-orbit splittings between Ψ_σ and Ψ_{HF} calculated for ^{16}O with the Kuo and the Sussex interactions are found to be smaller than their corresponding Tabakin values. These observations also hold in the case of ^{4}He for all the three interactions used. In the case of ^{40}Ca the single particle structure of the wave function Ψ_σ is hardly distinguishable from that of Ψ_{HF}.

Let us now consider the energy 'gaps' in the two variational solutions. This 'gap' is defined as the energy difference between the lowest unoccupied and the highest occupied s.p.energy levels. For the case of ^{16}O we find that with all the three interactions used, the variance minimization method produces a gap which is only slightly larger than the HF gap. The maximum gap difference of only 0.43 MeV is found in the calculation with the Kuo matrix elements.

We show in Tables III-7, III-8 and III-9 the single-particle wave functions for the interactions of Tabakin, Sussex and Kuo respectively. We have shown only the lowest $s_{1/2}$, $p_{3/2}$ and $p_{1/2}$ orbits (the others are either orthogonal to these or do not contain radial admixtures) and the expansion coefficients for these orbits in terms of pure harmonic oscillator (H.O.) basis wave functions (see Eq.IIC(3)). We see from the results that the variance minimization procedure generates s.p.orbitals which contain more admixture of H.O. radial wave functions than the HF procedure. This feature is common to all the nuclei studied with the three different interactions. This is due, partly, to the fact that besides 1ph, 2ph excitations are also included in the minimization of σ^2.

TABLE III-1

Some properties of $\Psi(\sigma^2)$ solution for spherical nuclei.
Calculation in 4 osc. major shells with cmm correction.
Interaction: Tabakin (b=1.81 fm for ^{4}He and ^{16}O. b=2.03 fm for ^{40}Ca)

Nucleus	$E(\sigma^2)$ (MeV)	E(2) (MeV)	E(Total) (MeV)	$r(\sigma^2)$ (fm)	$\alpha^{-2}(\sigma^2)$	Width (MeV)
^{4}He	-9.65	-2.96	-12.61	1.758	0.9730	11.72
^{16}O	-41.98	-10.66	-52.64	2.309	0.8752	23.08
^{40}Ca	-125.07	-15.87	-140.94	3.433	0.5550	21.29

TABLE III-2

Some properties of Ψ_σ^2 solution for spherical nuclei in 4 major oscillator shells.

Interaction: Sussex (b=1.7 fm) with cmm correction.

Nucleus	E(σ^2) (MeV)	E2(σ^2) (MeV)	E(Total) (MeV)	r(σ^2) (fm)	$\alpha^2(\sigma^2)$	Width σ (MeV)
^{4}He	-12.32	-3.79	-16.11	1.709	0.9665	14.91
^{16}O	-89.70	-11.19	-100.89	2.200	0.8894	25.98
^{40}Ca	-382.95	-18.61	-401.56	2.889	0.6690	30.14

TABLE III-3

Some properties of Ψ_{σ^2} solution for spherical nuclei in 4 major oscillator shells.

Interaction: Kuo bare ($\hbar\omega$ =12.5 MeV) with cmm correction

Nucleus	E(σ^2) (MeV)	E2(σ^2) (MeV)	E(Total) (MeV)	r(σ^2)	α^2(σ^2)	Width σ (MeV)
^{4}He	-24.24	-7.25	-31.49	1.746	0.9421	22.06
^{16}O	-166.44	-11.71	-178.15	2.209	0.9007	29.10
^{40}Ca	-550.89	-30.28	-581.17	3.047	0.5793	38.63

TABLE III-4

Interaction: Tabakin (b=1.81 fm for ^{4}He and ^{16}O. b=2.03 for ^{40}Ca) with cmm correction

Single particle energies (MeV)

		$s_{1/2}$	$p_{3/2}$	$p_{1/2}$	$d_{5/2}$	$s_{1/2}'$	$d_{3/2}$	$f_{7/2}$	$p_{3/2}'$	$f_{5/2}$	$p_{1/2}'$
^{4}He	HF	-19.27	7.45	9.12	17.33	12.83	20.55	25.82	23.34	28.39	28.18
	σ^2	-20.87	7.63	9.43	17.43	12.12	20.84	25.91	23.24	28.52	28.59
^{16}O	HF	-42.63	-19.79	-11.76	3.33	5.83	11.71	16.22	13.99	23.84	16.13
	σ^2	-46.06	-21.43	-11.91	3.38	6.12	12.59	16.35	13.69	24.39	15.91
^{40}Ca	HF	-52.53	-33.23	-27.11	-15.55	-12.02	-8.27	-3.99	1.56	3.85	4.31
	σ^2	-52.92	-33.45	-27.23	-15.57	-12.01	-8.22	-3.97	1.50	3.91	4.27

TABLE III-5

Interaction: Sussex (b=1.7 fm) with cmm correction

Single Particle Energies (MeV)

		$s_{1/2}$	$p_{3/2}$	$p_{1/2}$	$d_{5/2}$	$s_{1/2}'$	$d_{3/2}$	$f_{7/2}$	$p_{3/2}'$	$f_{5/2}$	$p_{1/2}'$
^4He	HF	-20.66	6.60	8.53	18.16	14.37	21.11	28.30	25.77	30.28	30.91
	σ^2	-22.49	6.80	8.85	18.27	13.51	21.40	28.46	25.47	30.46	31.46
^{16}O	HF	-52.79	-26.62	-19.55	-0.09	1.19	7.83	15.37	12.49	22.59	14.91
	σ^2	-56.11	-28.21	-19.86	-0.12	1.28	8.55	15.44	12.13	23.04	14.68
^{40}Ca	HF	-87.83	-57.51	-50.51	-30.92	-26.91	-21.17	-12.68	-4.73	-1.54	-0.71
	σ^2	-88.16	-57.69	-50.61	-30.95	-26.90	-21.11	-12.67	-4.77	-1.48	-0.75

TABLE III-6

Interaction: Kuo ($\hbar\omega$ = 12.5 MeV) with cmm correction

Single Particle Energies (MeV)

		$s_{1/2}$	$p_{3/2}$	$p_{1/2}$	$d_{5/2}$	$s_{1/2}'$	$d_{3/2}$	$f_{7/2}$	$p_{3/2}'$	$f_{5/2}$	$p_{1/2}'$
^{4}He	HF	-28.12	5.08	7.51	15.66	10.19	18.31	24.96	19.32	26.41	24.59
	σ^2	-29.62	5.39	7.83	15.87	9.49	18.58	25.14	19.15	26.53	25.11
^{16}O	HF	-68.60	-37.04	-28.29	-3.07	-1.51	4.72	12.36	8.52	18.68	9.81
	σ^2	-70.88	-38.05	-28.44	-2.79	-1.18	5.31	12.48	8.44	18.93	9.65
^{40}Ca	HF	-97.94	-66.53	-60.31	-35.06	-30.71	-26.81	-15.91	-9.58	-6.91	-6.83
	σ^2	-97.99	-66.54	-60.33	-35.06	-30.71	-26.80	-15.91	-9.58	-6.90	-6.84

TABLE III-7

Interaction: Tabakin (b = 1.81 fm for ^{4}He and ^{16}O. b = 2.03 for ^{40}Ca) with cmm correction

Single Particle Orbits (Expansion coefficients for the lowest three orbits shown)

		$S_{1/2}$		$P_{3/2}$		$P_{1/2}$	
		$0s_{1/2}$	$1s_{1/2}$	$0p_{3/2}$	$1p_{3/2}$	$0p_{1/2}$	$1p_{1/2}$
^{4}He	HF	0.9668	0.2554	0.9667	-0.2559	0.9310	-0.3649
	σ^2	0.9381	0.3461	0.9553	-0.2953	0.9098	-0.4148
^{16}O	HF	0.9860	0.1667	0.9787	0.2051	0.9910	0.1340
	σ^2	0.9729	0.2308	0.9563	0.2921	0.9712	0.2382
^{40}Ca	HF	0.9908	0.1351	0.9867	0.1625	0.9917	0.1288
	σ^2	0.9885	0.1510	0.9838	0.1791	0.9892	0.1465

TABLE III-8

Interaction: Sussex (b = 1.7 fm) with cmm correction

Single Particle Orbits (Expansion coefficients for the lowest three orbits shown).

		$S_{1/2}$		$P_{3/2}$		$P_{1/2}$	
		$0s_{1/2}$	$1s_{1/2}$	$0p_{3/2}$	$1p_{3/2}$	$0p_{1/2}$	$1p_{1/2}$
^4He	HF	0.9849	0.1728	0.9702	-0.2424	0.9321	-0.3622
	σ^2	0.9634	0.2680	0.9635	-0.2674	0.9149	-0.4036
^{16}O	HF	0.9877	0.1564	0.9837	0.1796	0.9920	0.1265
	σ^2	0.9767	0.2142	0.9656	0.2597	0.9775	0.2104
^{40}Ca	HF	0.9926	0.1216	0.9922	0.1246	0.9944	0.1060
	σ^2	0.9915	0.1296	0.9908	0.1349	0.9933	0.1154

TABLE III-9

Interaction: Kuo ($\hbar\omega$ = 12.5 MeV) with cmm correction.

Single Particle Orbits (Expansion coefficients for the lowest three orbits shown).

		$S_{1/2}$		$P_{3/2}$		$P_{1/2}$	
		$0s_{1/2}$	$1s_{1/2}$	$0p_{3/2}$	$1p_{3/2}$	$0p_{1/2}$	$1p_{1/2}$
^4He	HF	0.9431	0.3324	0.9935	-0.1138	0.9478	-0.3188
	σ^2	0.9057	0.4238	0.9869	-0.1609	0.9296	-0.3685
^{16}O	HF	0.9567	0.2912	0.9273	0.3744	0.9369	0.3495
	σ^2	0.9440	0.3298	0.9015	0.4326	0.9077	0.4194
^{40}Ca	HF	0.9756	0.2196	0.9635	0.2676	0.9647	0.2633
	σ^2	0.9743	0.2249	0.9629	0.2695	0.9649	0.2623

REFERENCES FOR CHAPTER III

1. V. Satyan and J.C. Parikh, in Proc. Nuclear Physics and Solid State Physics Symposium, Bangalore (1973), Vol.16B, p.134.

2. V. Satyan and J.C. Parikh, Physical Review C (to appear)

CHAPTER IV

WIDTHS OF DEFORMED HARTREE-FOCK STATES

A. INTRODUCTION

In this chapter we discuss the application of the concept of width as a measure for the goodness of Hartree-Fock states of deformed nuclei. Only those nuclei for which the assumption of axial symmetry seems to work well are studied here. This study forms a natural extension of our study of the goodness of HF states of spherical nuclei which was presented in Chapter II. Work on lines similar to ours described in this section has been reported by a few authors[1-4] earlier. Our purpose here in presenting this study on widths of deformed nuclei is two fold: first, for the sake of completeness of our discussion on widths it is necessary to include in our study a discussion on the widths of deformed nuclei. Secondly, we would like to present here some results of constrained HF and projection calculations for Preedom-Wildenthal and K+12FP interactions and also for a Schematic interaction which have not been reported so far in literature.

In section B of this chapter we discuss the concept of intrinsic wave function and the question what the width

of a deformed intrinsic state tells us. We point out there that the concept of width as a measure for goodness (as discussed in Chapter II) is useful only for those approximate wave functions which have exactly the same symmetries as the real eigenstates of the Hamiltonian. As for the concept of width applied to deformed intrinsic states it has a different meaning and use which we discuss in some detail in the same section. In Section C we describe a schematic interaction for the 0d-1s shell built on considerations of certain symmetries and energy systematics. This interaction is so constructed that it is exactly soluble and it gives exact rotational spectrum. By virtue of these properties this interaction is useful in testing HF approximation together with angular momentum projection. In Section D we describe HF plus angular momentum projection calculations for N=Z even-even nuclei in the 0d-1s shell using the schematic, the Preedom-Wildenthal and the K+12 FP interactions. The results of these calculations are discussed next.

B. DEFORMED HARTREE-FOCK STATES AND WIDTHS

We have already reviewed in Chapter II the Hartree-Fock method for obtaining approximate states. In this

section we consider its application to non closed shell nuclei.

It is well-known that there is a large class of nuclei which exhibit rotational properties at low excitation energies. Many attempts have been made to understand this rotational behaviour of highly deformed nuclei both from the phenomenological and the microscopic view points. The phenomenological model approach consists in using a moment of inertia to describe the states when the spectrum is rotational. On the other hand, the microscopic theories are based on the assumption that one can describe the states of a rotational band starting from a shell model single particle well plus a two-body interaction and then using Hartree-Fock or Hartree-Fock-Bogoliubov theories to obtain the 'best' approximations to the intrinsic wave function and finally employing a projection technique to project out the various good angular momentum states of the rotational band. It is this latter approach using the HF prescription that we have used in this section to study some nuclei in 0d-1s shell under the assumption of axial symmetry.

The concept of an intrinsic wave function has proved to be very useful in the theory of rotational nuclei. The

idea here is that in a highly deformed nucleus the low lying energy states can be considered compositely by a single deformed wave function called the intrinsic wave function and the states of good angular momentum projected from it describe well the actual eigenstates. Let Φ_K denote the intrinsic wave function and Ψ^J_{MK} the good angular momentum states projected from it. Then

$$\Psi^J_{MK} = \frac{2J+1}{C_{JK}\, 8\pi^2} \int d\Omega \; D^{J*}_{MK}(\Omega)\, R(\Omega)\, \Phi_K \qquad \text{IVB(1)}$$

Here $R(\Omega)$ is the operator of rotation through Euler angles Ω, $D^J_{MK}(\Omega)$ is a representation of $R(\Omega)$, J is the angular momentum and M its projection in the laboratory frame, K is the projection of J_Z on the Z-axis of the intrinsic frame, and C_{JK} is the normalization constant such that

$$\Phi_K = \sum_J C_{JK}\, \Psi^J_{MK} \qquad \text{IVB(2)}$$

with Φ_K and Ψ^J_{MK} normalized. It is assumed that the projected states Ψ^J_{MK} are eigenfunctions of the Hamiltonian H:

$$H \; |\Psi^J_{MK}\rangle = E_J \; |\Psi^J_{MK}\rangle \qquad \text{IVB(3)}$$

The HF procedure has been extensively used to obtain approximate intrinsic wave functions, i.e. one approximates Φ_K by a Slater determinant Φ^{HF}_K having the lowest energy:

$$\delta \frac{\langle \Phi_K | H | \Phi_K \rangle}{\langle \Phi_K | \Phi_K \rangle} = 0 \qquad \text{IVB(4)}$$

where δ denotes first order variations in Φ_K. In general the intrinsic wave function Φ^{HF}_K obtained by a HF variational calculation, will not be an eigenfunction of the Hamiltonian H. This is because, first, the HF determinant being an independent particle wave function is only an approximation to the correlated intrinsic wave function supposing that it exists. Secondly, a deformed intrinsic wave function cannot be used as an approximation to the eigenfunctions of H which have good J symmetry. The third reason is that even if Eq.IVB(3) is true, the eigenvalues E_I are in general nondegenerate. Therefore, a linear combination of the Ψ^J_{MK} will not be an eigenfunction of H.

The eigenvalues can be made degenerate by subtracting from the Hamiltonian H a polynomial operator $P(\vec{J}^2)$ of $\vec{J}^2$, where the polynomial P(J(J+1)) gives the dependence of E_J on J. Under the assumption that the states are rotational we have $P(\vec{J}^2) \sim \alpha \vec{J}^2$ where α is a parameter. We can write[1-2]

$$H_\alpha = H - \alpha \vec{J}^2 \qquad \text{IVB(5)}$$

Now by a suitable choice of the parameter α we can make the J-states of the band degenerate, i.e.

$$H_\alpha \left| \Psi^J_{MK} \right\rangle = E_\alpha \left| \Psi^J_{MK} \right\rangle \qquad \text{IVB(6)}$$

and

$$H_\alpha \left| \Phi_\alpha \right\rangle = E_\alpha \left| \Phi_\alpha \right\rangle \qquad \text{IVB(7)}$$

Eq.IVB(7) follows from the fact that a linear combination of Ψ^J_{MK} is also an eigenfunction of H_α. In Eq.IVB(5) the parameter α is related to the moment of inertia I of the band according to

$$\alpha = \frac{\hbar^2}{2I} \qquad \text{IVB(8)}$$

It is not essential that the intrinsic wave function should be an eigenfunction of H in order that its projections be eigenfunctions of H. But if Φ_α is an eigenfunction of H_α then we have that $\Psi^J_{MK}(\alpha)$ are eigenfunctions of H. We can see this as follows: we have

$$\Phi^\alpha_K = \sum_J C^\alpha_{JK} \Psi^\alpha_{JK}$$

$$\therefore H\Phi^\alpha_K = \sum_J C^\alpha_{JK} H \Psi^\alpha_{JK}$$

$$= \sum_J C^\alpha_{JK} (H_\alpha + \alpha J^2) \Psi^\alpha_{JK}$$

$$= \sum_J C^\alpha_{JK} \left[E^\alpha_J + \alpha J (J+1)\right] \Psi^\alpha_{JK}$$

Expanding Φ^α_K on the left side we get

$$\sum_J C^\alpha_{JK} H \Psi^\alpha_{JK} = \sum_J C^\alpha_{JK} \left[E^\alpha_J + \alpha J(J+1)\right] \Psi^\alpha_{JK}$$

from which it follows that

$$H \Psi^\alpha_{JK} = \left[E^\alpha_{JK} + \alpha J(J+1)\right] \Psi^\alpha_{JK}$$

The advantage in considering H_α instead of H is that it justifies the use of HF variational procedure to find Φ_α since in that case Eq.IVB(6) will be satisfied.

To determine the best Φ_α and the best value of the parameter α we first define the variance of Φ_α with respect to the Hamiltonian H_α :

$$\sigma^2(\Phi_\alpha) = \langle \Phi_\alpha | H_\alpha^2 | \Phi_\alpha \rangle - |\langle \Phi_\alpha | H_\alpha | \Phi_\alpha \rangle|^2$$

IVB(9)

Then in the ideal situation where $E_J = E_0 + \alpha J(J+1)$ and the good-J states projected from Φ_α are the corresponding eigenstates we would have $\sigma^2(\Phi_\alpha) = 0$. In practice, however, the best one can do is to minimize $\sigma^2(\Phi_\alpha)$ so as to get the best α and Φ_α . The procedure then is as follows: We choose a certain value for α , then carry out HF variational calculation to obtain the intrinsic wave function Φ_α and then we evaluate its width (Eq. IVB(9)). We repeat this procedure varying the parameter α until the minimum value of $\sigma^2(\Phi_\alpha)$ is found. Finally we project out good-J states from this minimum width intrinsic wave function Φ_α . The above method has the further advantage that it gives bounds for errors of the eigenvalues and thus indicates whether the assumption of axial symmetry is good or not (see Chapter II, Section A, for the discussion on bounds).

The concept of width of an intrinsic state introduced in Eq.IVB(9) should be clearly distinguished from the width of an approximate state of the Hamiltonian H introduced in Chapter II. This latter width is a measure of goodness of an approximation to an eigenstate of H and this approximate state has all the exact symmetries of the actual eigenstate. Only, it is an approximation. This was the situation with the spherical Hartree-Fock states whose widths we evaluated and discussed in Chapter II and further minimized in Chapter III. In this chapter we are dealing with intrinsic HF states which are deformed and as such these can never be used as approximations to the actual eigenstates of the Hamiltonian which have good J. The width defined in Eq.IVB(9) gives the error we have made in approximating the deformed intrinsic wave function Φ by the determinant Φ_α and to find the best α and Φ_α, we have to minimize this error. However, we can apply the concept of width as defined in Chapter II to the states of good-J projected from the intrinsic wave function i.e. we may define

$$\sigma^2(\Psi^J_{MK}) = \langle \Psi^J_{MK} | H^2 | \Psi^J_{MK} \rangle - |\langle \Psi^J_{MK} | H | \Psi^J_{MK} \rangle|^2$$

IVB(10)

It is possible to relate these variances for projected J states to the variance of the intrinsic wave function Φ_K defined with respect to H:

$$\sigma^2(\Phi_K) = \langle \Phi_K | H^2 | \Phi_K \rangle - |\langle \Phi_K | H | \Phi_K \rangle|^2 \qquad \text{IVB(11)}$$

With the variance defined as in Eq.IVB(10) for a projected J-state it is then straightforward to consider its application to the deformed nuclei in exactly the same way as was done for spherical nuclei in Chapters II and III. However, these are aspects which we have not considered here.

C. A SCHEMATIC INTERACTION FOR THE 0d-1s SHELL

We described in the previous section a method for obtaining good approximations to the intrinsic wave function for highly deformed nuclei. We describe in this section a schematic[5] Hamiltonian in the 0d-1s shell which when used in conjunction with the above method yields very good intrinsic states. This interaction has been so constructed that it is exactly soluble and gives pure rotational spectrum for nuclei in 0d-1s shell. Hence we can use this interaction to illustrate the method we have discussed in the previous section.

The interaction part of the schematic Hamiltonian is chosen to be of the following form:

$$V_2 = \sum_{ij} V_{ij} = A\binom{n}{2} + B\,G(SU(6)) + C\,G(SU(3)) + D\vec{L}^2 + E\vec{S}^2 + F_1\vec{J}^2 + F_2\vec{T}^2$$

IVC(1)

where A, B, C, D, E, F_1, F_2 are coefficients to be determined and n is the number operator. The Casimir operators $G(SU(6))$ and $G(SU(3))$ have the well-known forms:

$G(SU(6)) \equiv M = \sum_{ij} P_{ij}$, the space-exchange Majorana operator

$$G(SU(3)) = \frac{3}{4}\vec{L}^2 + \frac{1}{4}Q\cdot Q$$

IVC(2)

where $\vec{L}$ is the orbital angular momentum operator and Q is the quadrupole operator. It is clear that V_2 preserves space symmetry, SU(3) symmetry, and L, S, J, T symmetries. Now the standard way of labelling the representations of U(6) and SU(3) is as follows:

Representation of U(6) : $[f] = [f_1 \ldots . f_6]$

Representation of SU(3): $(\lambda\mu)$

IVC(3)

The expectation values of the Casimir operators in these representations are given by

$$\langle G(SU(6)) \rangle_{[f]} = \tfrac{1}{2} \sum_{i=1}^{6} f_i (f_i - 2i + 1) \qquad \text{IVC(4)}$$

$$\langle G(SU(3)) \rangle_{(\lambda\mu)} = (\lambda+\mu)(\lambda+\mu+3) - \lambda\mu \qquad \text{IVC(5)}$$

The coefficient A in Eq.IVC(1) represents the average nucleon nucleon interaction. Coming to the one-body part of the Hamiltonian this has the following form:

$$V_1(\text{one-body}) = 10C + D\, l(l+1) + \tfrac{3}{4} E + F_1 j(j+1) + F_2 s(s+1)$$

IVC(6)

The parameters C, D, E, F_1 and F_2 are the same as those in Eq.IVC(1).

The parameters A, B,.....F_2 in Eq.IVC(1) are chosen so that,

i) the binding energies of the nuclei come out reasonably well.

ii) the centroid spacings of SU(6) representations correspond to those given by a 'realistic' two-body interaction.

iii) the centroid spacings of SU(3) representations contained in the lowest SU(6) representation is roughly what one expects from the assignments of SU(3) representations to levels in ^{20}Ne.

iv) the coefficients of $\vec{L}^2$, $\vec{S}^2$, $\vec{J}^2$ and $\vec{T}^2$ are chosen in such a way that the

(a) states of lower J lie lower in energy

(b) for (4n+2) nuclei the $T_<$ states in the maximum space symmetry representation are lower in energy by about 2 MeV than $T_>$ states.

We give below several useful numbers for this interaction:

(i) $E(2^+)-E(0^+)=1.5$ MeV for all even even N=Z nuclei

(ii) $E_c([f]_{(max-1)})-E_c([f]_{max}) = +7.2$ MeV

Here $[f]_{max}$ is the leading SU(6) representation and $[f]_{(max-1)}$ the next lower symmetry.

(iii) $E_c((\lambda\mu)=(42)) - E_c((\lambda\mu)=(80)) = 8.4$ MeV

From the above mentioned considerations it turns out that the coefficients $A, B, \ldots\ldots F_2$ in Eq.IVC(1) have the following values:

$$\begin{aligned} A &= -2.00 \text{ for } {}^{20}Ne \\ &\quad -1.55 \text{ for } {}^{24}Mg \\ &\quad -1.35 \text{ for } {}^{28}Si \\ B &= -1.8 \\ C &= -0.2 \\ D &= -0.35 \\ E &= 1.08 \\ F_1 &= 0.6 \\ F_2 &= 2.67 \end{aligned} \qquad \text{IVC(8)}$$

Since A varies from nucleus to nucleus the first term in Eq.IVC(1) contains many-body effects. Substituting the values of the coefficients from Eq.IVC(8) we get

$$V_2 = A\binom{n}{2} - 1.8\, G(SU(6)) - 0.2\, G(SU(3)) - 0.35\, \vec{L}^2 + 1.08\, \vec{S}^2 + 0.6\vec{J}^2 + 2.67\vec{T}^2 \qquad \text{IVC(9)}$$

and the one-body energies (Eq.IVC(6)) are:

$$\epsilon(0d_{5/2}) = 3.96 \text{ MeV}$$
$$\epsilon(1s_{1/2}) = 1.26 \text{ MeV} \qquad \text{IVC(10)}$$
$$\epsilon(0d_{3/2}) = 0.96 \text{ MeV}$$

Note the queer sequence of d-levels. For a given nucleus it is easy to calculate the energies of its states from a knowledge of the representations $[f]$ and $(\lambda\mu)$ and the values of the quantum numbers L, S, J and T. The wave functions for the states follow from the representations used. Thus this interaction is exactly soluble and yields J(J+1) spectrum for the nuclei.

D. NUMERICAL RESULTS AND DISCUSSION

In this section we describe some of our HF and width calculations and results for N=Z even even nuclei in the 0d-1s major shell using the method described in Section B.

We show in Table IV-1 the results of deformed HF calculations in 0d-1s shell for the nuclei ^{20}Ne, ^{28}Si and ^{36}Ar. The assumption of axial symmetry has been made. These calculations have been done using the Schematic[5] interaction described in the previous section. In Table IV-1 the second column shows α the moment of inertia

parameter (Eq. IVB(8)), the third column gives the energy of the intrinsic state Φ_α and the fourth column the expectation value of the quadrupole operator in the state Φ_α. The σ^2 in the fifth column is the variance of the HF state with the Hamiltonian H_α (Eq. IVB(9)). In the last column is shown the HF gap which is defined as the energy difference between the highest occupied and the lowest unoccupied levels in the HF single-particle spectrum.

We see that the schematic interaction gives large values for widths for the nuclei listed when an unmodified Hamiltonian is used ($\alpha = 0$). The HF gaps are twice as large as what one usually finds (~ 8 MeV) with realistic interactions in the 0d-1s shell (see Tables IV-2 and IV-3). We find that the widths and HF gaps of ^{20}Ne and ^{36}Ar are the same which indicates that there is a particle-hole symmetry for widths and HF gaps with the schematic interaction. Coming to the discussion on results with the modified Hamiltonian H_α we observe that the widths of HF states of all the nuclei shown are zero. Thus we have here intrinsic states which represent bands of collapsed J-states and hence these intrinsic states as well as their projected states are eigenstates of the Hamiltonian H. Further we note that the moment of inertia parameter α is the same for all the three nuclei. This value of $\alpha = 0.25$ is considerably

larger than the values of α one usually finds for ^{20}Ne and ^{28}Si. We show in Table IV-4 the spectrum of the ground state band of J-states. The second column in Table IV-4 shows the energies of the J-states projected from the $\alpha = 0$ HF solution and the third column shows the same for $\alpha = 0.25$ HF solution. The last column gives the exact spectrum (see the previous section). We see that the spectrum projected from $\alpha = 0$ HF intrinsic state is already close to being a J(J+1) spectrum. With the modified Hamiltonian H_α ($\alpha = 0.25$) we get a pure J(J+1) spectrum which is identical with the exact spectrum.

Let us now consider the results of our calculations done using the Preedom-Wildenthal[6] interaction. This two-body interaction is a modification of the well-known Kuo[8] interaction in the 0d-1s shell and gives good fit to the experimental data for nuclei in the mass region A=18-22. The complete Hamiltonian consists of 63 two-body matrix elements plus the 3 single particle energies viz. $(0d_{5/2}) = 0.0, (1s_{1/2}) = 0.87$ MeV and $(0d_{3/2}) = 5.08$ MeV. We show in Table IV-2 results of HF calculations for ^{20}Ne, ^{28}Si and ^{36}Ar. Considering first the results of unconstrained calculations ($\alpha = 0$) we see that the HF solutions of ^{20}Ne, ^{28}Si are quite stable as indicated by their large HF gaps. The HF gap in ^{36}Ar is small. The width in all the

cases is fairly large. We next investigate the contribution to the widths coming from the non-degeneracy of the J-levels in the spectrum.

Table IV-2 also shows the results of constrained HF calculations ($\alpha \neq 0$). We find that the widths are considerably reduced when α is varied. But the minimum widths are not close to zero which may be taken as an indication that the assumption of $J(J+1)$ sequence for the HF projected spectrum is not good and/or that the Slater determinantal HF description of the intrinsic states is inadequate. In the case of all the nuclei listed (Table IV-2) the HF gaps for the two HF solutions i.e. for $\alpha = 0$ and $\alpha \neq 0$ turn out to be nearly equal. We next show in Tables IV-5 and IV-6 the J-projected spectra of ^{20}Ne, ^{28}Si and ^{36}Ar using the HF solutions shown in Table IV-2. The absolute energies of the 0^+ states are shown in brackets in Tables IV-5 and IV-6. The energies of the excited states of the ground state band are shown relative to the 0^+ state which is taken as zero. The projected ground state of ^{20}Ne from the HF solution for $\alpha = 0.177$ shows a definite improvement over the one projected from $\alpha = 0$ solution. For comparison the experimental numbers are shown in the last column of Table IV-5. There is a similar marked improvement in the case of ^{28}Si and ^{36}Ar when the

modified Hamiltonian is used (Table IV-6).

The results of calculations done using the K+12FP[7] interaction are presented in Tables IV-3, IV-7 and IV-8. The K+12FP Hamiltonian is a modification of the Kuo effective Hamiltonian for the 0d-1s shell and has been adjusted to fit the ground state binding energies and level excitations in the nuclei A=17-22. The adjusted parameters in this Hamiltonian are the three single particle energies plus nine two-body matrix elements involving only $0d_{5/2}$ and $1s_{1/2}$ orbits. All other two-body matrix elements are held fixed at the Kuo[8] values. The K+12FP results for ^{20}Ne are similar to the results obtained with Preedom-Wildenthal (PW) interaction. The moment of inertia is the same as in the case of PW interaction but the minimum width is larger than the PW width. If we look at the projected spectrum of ^{20}Ne (Table IV-7) the $\alpha = 0.177$ HF projected spectrum is definitely better than the ordinary ($\alpha = 0$) HF projected spectrum except for the 4^+ state. In the case of ^{28}Si the lowest HF solution is oblate and has a large width. When α is varied the width reduces substantially but the absolute magnitude of the minimum width still remains large. The projected spectrum of ^{28}Si (Table IV-7) obtained from $\alpha = 0.16$ HF intrinsic state shows a slight improvement

over the α = 0 spectrum in that with α = 0.16, the energy of the 0^+ state is lowered a little. The large intrinsic width with α = 0.16 and only slight improvement in the 0^+ energy with α = 0.16 essentially imply that the single determinant assumption does not work well for ^{28}Si with the K+12FP Hamiltonian. In the case of ^{36}Ar also (Tables IV-3 and IV-8) we find that α = 0 HF projected ground state is better than the projected J = 0 state obtained from the constrained HF solution (α = 0.23).

TABLE IV-1

Some properties of deformed HF states of even-even N=Z 0d-1s shell nuclei with the Hamiltonian $H_\alpha = H - \alpha J^2$.

Interaction: Schematic

S.P.Energies (MeV): $(0d_{5/2})$=3.96, $(1s_{1/2})$=1.26, $(0d_{3/2})$=0.96.

Nucleus	α	Energy (MeV)	$\langle Q20 \rangle$	σ^2	HF gap (MeV)
^{20}Ne	0.0	-36.71	+15.78	12.56	16.97
	0.25	-36.40	+16.00	0.0	17.34
^{28}Si	0.0	-130.10	+23.90	35.61	18.47
	0.25	-129.91	+24.00	0.0	18.41
^{36}Ar	0.0	-229.19	-15.72	12.59	16.97
	0.25	-228.96	-16.00	0.0	17.34

TABLE IV-2

Some properties of deformed HF states of even-even N=Z 0d-1s shell nuclei with Hamiltonian $H_\alpha = H - \alpha J^2$.
Interaction: Preedom-Wildenthal.
S.P. Energies (MeV): $(0d_{5/2})=0.0$, $(1s_{1/2})=0.87$, $(0d_{3/2})=5.08$.

Nucleus	α	Energy (MeV)	$\langle Q20 \rangle$	σ^2	HF gap (MeV)
^{20}Ne	0.0	-20.01	+15.31	13.79	7.27
	0.177	-19.90	+14.96	4.87	7.21
^{28}Si	0.0	-82.01	-19.79	46.17	9.18
	0.21	-81.77	-20.42	16.35	8.83
^{36}Ar	0.0	-142.75	-9.46	30.57	3.63
	0.35	-141.79	-11.94	10.09	3.68

TABLE IV-3

Some properties of deformed HF states of even-even N=Z 0d-1s shell nuclei with the Hamiltonian $H_\alpha = H - \alpha J^2$.

Interaction: K+12 FP

S.P.Energies (MeV): $(0d_{5/2})=0.0$, $(1s_{1/2})=0.90$, $(0d_{3/2})=5.75$.

Nucleus	α	Energy (MeV)	$\langle Q20 \rangle$	σ^2	HF gap (MeV)
^{20}Ne	0.0	-19.41	+15.56	13.61	7.04
	0.177	-19.29	+15.20	5.23	6.97
^{28}Si	0.0	-87.29	-23.00	32.36	9.67
	0.16	-87.16	-22.88	13.56	9.62
^{36}Ar	0.0	-177.78	-15.34	15.80	7.52
	0.23	-177.57	-15.58	5.39	8.77

TABLE IV-4

HF projected spectra of ^{20}Ne with the Hamiltonian $H_\alpha = H - \alpha J^2$

Interaction: Schematic.

S.P. Energies (MeV): $(0d_{5/2})=3.96$, $(1s_{1/2})=1.26$, $(0d_{3/2})=0.96$

K=0 (Prolate solution) (All energies are in MeV)

J^π	$\alpha = 0$ E_J(HF)	$\alpha = 0.25$ E_J(HF)	E_J(Exact)
0^+	-39.97	-40.40	-40.40
2^+	-38.56	-38.90	-38.90
4^+	-35.21	-35.40	-35.40
6^+	-29.82	-29.90	-29.90
8^+	-22.15	-22.28	-22.40

TABLE IV-5

HF projected spectra of ^{20}Ne with the Hamiltonian $H_\alpha = H - \alpha J^2$

Interaction: Preedom-Wildenthal.

S.P. Energies (MeV): $(0d_{5/2})=0.0$, $(1s_{1/2})=0.87$, $(0d_{3/2})=5.08$

K=0 (Prolate solution) (All energies are in MeV)

J^π	$\alpha=0$ E_J(HF)	$\alpha=0.177$ E_J(HF)	E_J(Expt)[a]
0^+	0.00(-23.24)	0.00(-23.45)	0
2^+	1.24	1.37	1.63
4^+	3.87	3.82	4.25
6^+	8.09	8.29	8.79
8^+	12.01	12.35	11.99

[a] Ref. 9.

TABLE IV-6

HF Projected spectra with the Hamiltonian $H_\alpha = H - \alpha J^2$
Interaction: Preedom-Wildenthal
S.P.Energies (MeV): $(0d_{5/2})=0.0$, $(1s_{1/2})=0.87$, $(0d_{3/2})=5.08$

Nucleus	^{28}Si			^{36}Ar			
	K=0 (Oblate solution)			K=0(Oblate solution)			
	$\alpha=0$	$\alpha=0.21$		$\alpha=0$	$\alpha=0.35$		
J^π	E_J(HF)	E_J(HF)	E_J(Expt)[a]	J^π	E_J(HF)	E_J(HF)	E_J(Expt)[b]
0^+	0.00(-86.37)	0.00(-86.62)	0	0^+	0.00(-144.09)	0.00(-144.65)	0
2^+	1.60	1.58	1.78	2^+	1.17	1.93	1.97
4^+	4.72	4.72	4.62	4^+	2.74	5.44	4.42
6^+	9.46	9.50	8.55	6^+	8.42	11.81	--
8^+	15.40	15.63	15.19(8^+)				

a) Ref.10
b) Ref.11

TABLE IV-7

HF projected spectra with the Hamiltonian $H_\alpha = H - \alpha J^2$

Interaction: K+12FP

S.P.Energies (MeV): $(0d_{5/2})=0.0$, $(1s_{1/2})=0.90$, $(0d_{3/2})=5.75$

Nucleus	^{20}Ne			^{28}Si			
	K=0(Prolate solution)			K=0(Oblate solution)			
	$\alpha=0$	$\alpha=0.177$			$\alpha=0$	$\alpha=0.16$	
J^π	E_J(HF)	E_J(HF)	E_J(Expt)[a]	J^π	E_J(HF)	E_J(HF)	E_J(Expt)[b]
0^+	0.00(-22.66)	0.00(-22.81)	0.00	0^+	0.00(-91.31)	0.00(-91.34)	0.00
2^+	1.27	1.37	1.63	2^+	1.08	1.06	1.78
4^+	4.00	3.82	4.25	4^+	3.59	3.52	4.62
6^+	8.04	8.16	8.79	6^+	7.44	7.30	8.55
8^+	11.57	11.82	11.99	8^+	12.36	12.17	15.19(8^+)

a. Ref.9

b. Ref.10

TABLE IV-8

HF projected spectra with the Hamiltonian $H_\alpha = H - \alpha J^2$

Interaction: K+12 FP

S.P.Energies (MeV) $(0d_{5/2})=0.0$, $(1s_{1/2})=0.90$, $(0d_{3/2})=5.75$

Nucleus	^{36}Ar		
K=0 (Oblate solution)			
J^π	$\alpha=0$ E_J(HF)	$\alpha=0.23$ E_J(HF)	E_J(Expt)[a]
0^+	0.00(-180.50)	0.00(-180.65)	0
2^+	1.50	1.28	1.97
4^+	4.45	4.25	4.42
6^+	7.96	8.69	--
8^+	8.80	11.36	--

a. Ref. 11

REFERENCES FOR CHAPTER IV

1. T.H.R. Skyrme, Proc. Phys. Soc. (London) A70, 433 (1957).
2. C.A. Levinson, Phys. Rev. 132, 2184 (1963).
3. M.K. Banerjee, D'Oliveira and Stephenson, Phys. Rev. 181, 1404 (1969).
4. J.C. Parikh and J.P. Svenne, Phys. Rev. C6, 34 (1972).
5. J.C. Parikh, private communication.
6. M. Preedom and B.H. Wildenthal, Phys. Rev. C6, 1633 (1972).
7. E.C. Halbert et al 'Advances in Nuclear Physics', Vol.4, Chapter 6, edited by M. Baranger and E. Vogt, Plenum Press (1971).
8. T.T.S. Kuo, Nucl. Phys. A103, 71 (1967).
9. J.A. Kuehnen and R.W. Ollerhead, Phys. Letts. 20, 301 (1966).
10. M. Soyeur and A.P. Zuker, Phys. Letts. 41B, 135 (1972).
11. M.A. Moinester and W.P. Alford, Nucl. Phys. A145, 143 (1970).
12. A. Graue et al, Nucl. Phys. A120, 513 (1968); G.T. Garve et al, Phys. Letts. 29B, 108 (1969); H. Nann and B.H. Wildenthal, Phys. Rev. C13, 1009 (1976).

CHAPTER V

UNITARY GROUPS AND OPERATOR NORMS

A. INTRODUCTION

Our study so far was centred mainly around wave functions and in particular with widths of determinantal wave functions and the variational method based on the minimization of width of a determinantal wave function. In this chapter we are concerned with fermion operators and spaces, and with measures for the "sizes" of operators in these spaces. We study these things from a group theoretic standpoint.

We will always be dealing with shell-model like spectroscopic spaces, and hence we will have a finite number N of s.p. basis states amongst which m nucleons are distributed. In such spectroscopic spaces it is clear that the unitary group U(N) is the starting point for discussion of the transformation properties of operators as well as states. Further, the various subgroups of U(N) provide additional frameworks for a more detailed study of these transformation properties. The subgroup we consider here is the direct sum subgroup $U(m)+U(N-m)$ of U(N) resulting from the decomposition of the N s.p. states into m occupied

and (N-m) unoccupied ones. Thus the unitary group point of view provides a natural mathematical framework for the study of the structures of operators and spaces and as we shall see later also for tackling some other physically relevant questions. We have therefore classified here the two-body interaction operator according to its transformation properties under U(N) and its direct sum subgroup $U(m)\dot{+}U(N-m)$.

In addition to classifying operators according to unitary groups it is also necessary for our purpose to be able to evaluate the sizes of operators in many particle spaces. As a proper measure for the size of an operator we consider here its Euclidean norm[1]. This is a proper measure in the sense that it satisfies all the mathematical conditions of a norm and further it is compatible with unitary norm used for wave functions of a system. We give the definition and properties of the Euclidean norm in Section B and also describe methods for its evaluation in many particle spaces.

In Section C we describe the classification of fermion operators under the group U(N). Techniques[4-6] for the U(N) decomposition of a general fermion operator are discussed here in some detail. These ideas are then extended in Section D to the case of decomposition of a

fermion operator under the direct sum subgroup $U(m)\dot{+}U(N-m)$.

We discuss in Section E the connection between the unitary groups and the HF approximation[6,8]. In the same section we carry out the decomposition of the two-body interaction into its irreducible tensor parts under the transformations of the subgroup $U(m)\dot{+}U(N-m)$ generated by the HF procedure. Our main aim in doing this is to find out how much of the higher unitary rank part of the interaction gets reduced to its lower rank parts under the transformations of the subgroup $U(m)\dot{+}U(N-m)$ when a HF calculation is done. More precisely, we want to find out the effective total one-body operator (i.e. operator of unitary rank $\overrightarrow{\nu} = (0+1)$ under $U(m)\dot{+}U(N-m)$) that is generated in the HF procedure and evaluate its norm in m particle spaces. We derive a polynomial expression for the square of norm of this operator in m particle spaces. This norm compared with the norm of the irreducible $\nu = 2$ rank part of the interaction under U(N) tells us to what extent the HF procedure has converted the U(N) irreducible $\nu = 2$ part of the interaction into an effective one-body operator under the subgroup $U(m)\dot{+}U(N-m)$. For this purpose we define an efficiency measure R as a ratio of norms of tensor components of interaction under U(N) and its subgroup. This ratio, as we shall see later, provides

us with a measure of the global goodness of the HF s.p. basis. We evaluate this ratio R for N=Z even even nuclei of 0f-1p and 0d-1s shells using realistic interactions. We describe these calculations in Sections F and G and also discuss the results of these calculations.

B. NORMS OF OPERATORS

In this section we consider the concept of norm as a measure of the size of an operator and discuss its uses and methods of its evaluation in many particle spaces[1-3].

Consider a general operator F and a space $\underset{\sim}{\alpha}$ in which it operates. Then a measure of the size of the operator F in $\underset{\sim}{\alpha}$ can be had by assigning to F a real number called norm of F in $\underset{\sim}{\alpha}$ which we denote by $||F||_{\underset{\sim}{\alpha}}$. The norm must satisfy the following conditions.

1. $||F|| \geq 0$; $||F|| = 0$ only for the null operator.
2. $||FG|| \leq ||F|| \cdot ||G||$ for any two operators F and G.
3. $||F+G|| \leq ||F|| + ||G||$ equality holds only if G=F.
4. $||kF|| = |k| \, ||F||$ where k is a constant.

A further requirement for the norm of an operator to be a proper measure of its size is that it should be compatible with the unitary norm (vector norm) which one usually uses for the state vectors of the system. That is,

$$||F\Psi|| \leq ||F|| \times ||\Psi|| \qquad \text{VB(1a)}$$

where the unitary norm is taken for $F\Psi$ and Ψ and the operator norm for $||F||$. In practice, a prescription is needed to calculate the norm of an operator in a given space. A suitable prescription for the measure of the size of an operator is the Euclidean norm defined by

$$\left\{ ||F||_{\underset{\sim}{\alpha}} \right\}^2 = \text{Trace}\,(F^+F)_{\underline{\alpha}} \qquad \text{VB(2)}$$

where F^+ is the adjoint of F. Since the trace in Eq.VB(2) is invariant under all unitary transformations of a given basis in the space, it follows that the Euclidean norm is a property of the operator and the space but not of any representation therein. It is easy to see that the Euclidean norm satisfies all the mathematical conditions for a norm listed in Eq.VB(1) together with Eq.VB(1a) by going over to the representation in which F is diagonal. We have

$$||F||^2_{\underset{\sim}{\alpha}} = \sum_i \lambda_i^2$$

where λ_i are the eigenvalues of F and $\sum \lambda_i^2$ satisfies all the conditions for the norm. The norm which we use in this chapter is, however, not the trace (Eq.VB(2)) but instead the average of F^+F in the space $\underset{\sim}{\alpha}$ i.e. we define

$$\left\{ ||F||_{\underset{\sim}{\alpha}} \right\}^2 = \langle F^+F \rangle^{\underset{\sim}{\alpha}} = \frac{1}{d(\underset{\sim}{\alpha})} \left[\mathrm{Tr}(F^+F)_{\underset{\sim}{\alpha}} \right] = \frac{1}{d(\underset{\sim}{\alpha})} \left(||F||_{\underset{\sim}{\alpha}} \right)^2 \qquad \text{VB(3)}$$

where $d(\alpha)$ is the dimensionality of the space $\underset{\sim}{\alpha}$. This is a slightly different definition of the norm but since $\left[\frac{1}{d(\underset{\sim}{\alpha})} \left(||F||_{\underset{\sim}{\alpha}} \right)^2 \right]^{1/2}$ gives the r.m.s. matrix element of the operator F in the space $\underset{\sim}{\alpha}$, it is a suitable measure of the size of F in $\underset{\sim}{\alpha}$.

The Euclidean norm also defines for us the orthogonality of the operator in $\underset{\sim}{\alpha}$. Two operators F and G are said to be orthogonal in $\underset{\sim}{\alpha}$ if

$$\langle FG \rangle^{\underset{\sim}{\alpha}} = 0. \qquad \text{VB(4)}$$

Further, two different symmetry components F_ν and $F_{\nu'}$ of the same operator F where ν and ν' are symmetry labels, are said to be orthonormal in the space $\underset{\sim}{\alpha}$ if

$$\langle F_\nu F_{\nu'} \rangle^{\alpha} = \delta_{\nu\nu'}$$

VB(5)

It has been shown by French[2] that the calculation of the Euclidean norm of an operator, say of the Hamiltonian H in the m-particle space, need not involve the evaluation of the matrix elements of H^+H in m-particle state functions. This is because the norm (its square, to be precise) being an average over all m-particle states, can be expressed as a polynomial of order u in the particle number m, where u is the maximum particle rank of the operator H^+H. This norm-polynomial is simply a Lagrange interpolation polynomial and can be expressed in the following form:

$$\langle H^+H \rangle^m = \sum_{s=0}^{u} \binom{u-m}{u-s} \binom{m}{s} \langle H^+H \rangle^s$$

$$= \sum_{s=0}^{u} (-1)^{s-u} \binom{m-s-1}{u-s} \binom{m}{s} \langle H^+H \rangle^s$$

$$\equiv \sum_{s=0}^{u} \rho_u(ms) \langle H^+H \rangle^s$$

VB(6)

Eq.VB(6) expresses the average $\langle H^+H\rangle^m$ in terms of its averages $\langle H^+H\rangle^s$ in s=0,1,2,.....u particle spaces which is the defining space of the operator H^+H. These $\langle H^+H\rangle^s$ averages are called 'input averages' and (u+1) such input pieces of information are required to completely specify the polynomial since it is of order u. In Eq.VB(6) the coefficient $\zeta_u(ms)$ is the projection operator for m=s particle space and it is zero for other m values in the defining space. In the case when H is a (0+1+2)-body operator we have that H^+H is of maximum particle rank 4. Then we get from Eq.VB(6) a 4^{th} order polynomial for $\langle H^+H\rangle^m$ expressed in terms of its values in s=0,1,2,3,4 particle-spaces. It is clear that this polynomial form requires input averages of $\langle H^+H\rangle^s$ for s=3 and 4 particle spaces which are often hard to evaluate. However, we can avoid this difficulty if we consider input averages in 0 and 1 hole spaces - i.e. $\langle H^+H\rangle^s$ with s=N and s=N-1 instead of the averages in s=3 and 4 particle spaces. The advantage here is that it is much easier to obtain these hole averages than the s=3,4 particle averages. In short, to fix a 4^{th} order polynomial we should know its values at (4+1) independent points and it is most economical to choose these values at the points s=0,1,2,and N-1, N.

Similarly in the general case also one can include hole spaces in the propagation formula and obtain the expression

$$\langle H^{+}H\rangle^{m} = \binom{N-m}{u_2+1} \sum_{s=0}^{u_1} (-1)^{s-u_1} \binom{N-s}{u_2+1}^{-1} \binom{m-s-1}{u_1-s}\binom{m}{s}\langle H^{+}H\rangle^{s}$$

$$+\binom{m}{u_1+1} \sum_{s=0}^{u_2} (-1)^{s-u_2} \binom{N-s}{u_1+1}^{-1} \binom{N-m-s-1}{u_2-s} \binom{N-m}{s} \langle H^{+}H\rangle^{s}$$

VB(7)

with $u_1+u_2 = u-1$. In Eq.VB(7) the defining space of the operator $H^{+}H$ consists of $s=0,1,2,\ldots.u_1$ particle spaces and $s=0,1,2,\ldots.u_2$ hole spaces.

In the following sections we consider the evaluation of the norm of H(2), the two-body interaction part of H, in m-particle spaces. For this purpose and also to study some questions relating to the HF approximation, we consider first the decomposition of H(2) according to the irreducible symmetries of the group U(N) and also of its subgroup $U(m)\dot{+}U(N-m)$.

C. DECOMPOSITION OF OPERATORS ACCORDING TO THE GROUP U(N)

We consider in this section the decomposition of a general operator according to the symmetries of the group $U(N)$[4-6].

We consider a set of N single-particle states which forms a basis in an N-dimensional vector space. The set of all unitary transformations in this space forms a group viz. the unitary group U(N). The group algebra can be described conveniently in terms of a set of N^2 infinitesimal operators $U_{ij}(i,j=1,....N)$ which form a linearly independent complete set. These operators are closed under commutation i.e.

$$\left[U_{ij}, U_{kl}\right] = U_{il}\,\delta_{jk} - U_{kj}\,\delta_{il} \qquad \text{VC(1)}$$

The N^2 operators U_{ij} are known as the infinitesimal operators of the group U(N). In the second quantization formalism the infinitesimal operators may be expressed in terms of products of anticommuting fermion creation and destruction operators A and B for the single-particle states. More precisely, the N^2 operators $U_{ij} = A_i B_j$, $i,j=1,....N$ are the infinitesimal generators of U(N) since

$$\left[U_{ij},U_{kl}\right] = \left[A_i B_j,\ A_k B_l\right] = U_{il}\ \delta_{jk} - U_{kj}\ \delta_{il}$$

VC(2)

where the last step follows from the anticommutation relations for A_i, B_j etc.

We next consider the transformation properties of operators under U(N). We confine our discussion to the class of fermion operators and fermion spaces only. The fundamental operators here are the creation and destruction operators A_i and B_i respectively for the single-particle states. Since the vaccum state of no particles and the closed-shell state of N-particles are both invariants under unitary transformations, it follows that the creation operator A_i transforms as a single-particle state and the destruction operator B_i as a one-hole state. Thus in terms of Young shapes[12] we have

$$A \equiv \{A_i\} \sim \square = [1]$$

$$B \equiv \{B_i\} \sim \left.\begin{array}{c}\square\\ \vdots\\ \square\end{array}\right\}_{N-1} = [1^{N-1}]$$

VC(3)

where $\sim$ means "transforms as". In general, for a k-body creation operator Z(k) which is a product of k A's we obtain, using Littlewood's rules[12] and taking account of the Pauli principle which allows for only the completely antisymmetrized representation,

$$Z(k) = A \times A \times \ldots . \times A \sim \left.\begin{array}{|c|}\hline \\ \hline \\ \hline \\ \hline \\ \hline \\ \hline \end{array}\right\}_{k} = [1^k]$$

(k factors)

VC(4)

and for the destruction operator $Z^+(k)$

$$Z^+(k) = B \times B \times \ldots . \times B \sim \left.\begin{array}{|c|}\hline \\ \hline \\ \hline \\ \hline \\ \hline \\ \hline \end{array}\right\}_{N-k} = [1^{N-k}]$$

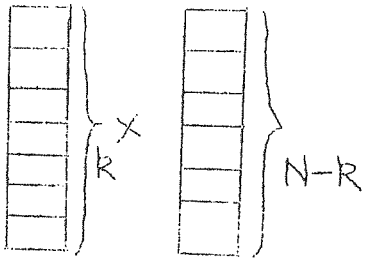
(k factors)

VC(5)

Now, considering general operators F, these are all contained in the set $\{Z(k)\ Z^+(k')\}$ of dimensionality 2^{4N}, where N is the total number of s.p. states. Since our concern here is with representations of operators under U(N), we need to consider only the number conserving operators. An operator F is said to be number conserving if

$$\left[g(n),F\right] = 0 \qquad \text{VC(6)}$$

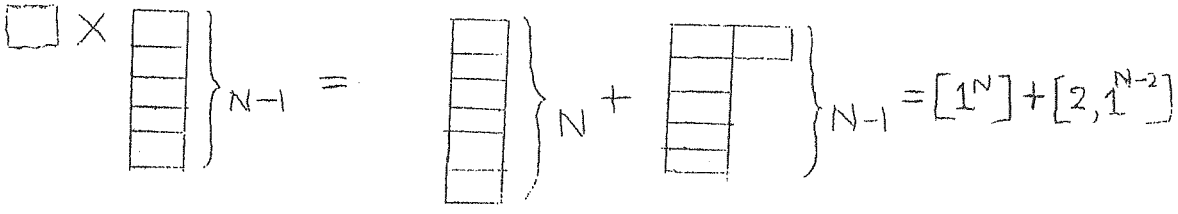
where $g(n)$ is a function of the number operator $n = \sum_{i=1}^{N} A_i B_i$. All number conserving operators are contained in the set $\left\{Z(k)\ Z^{+}(k)\right\}_{\text{all } k}$. Then to find out how a k-body operator F of the above type transforms under U(N) we have to consider first how the product $Z(k)Z^{+}(k)$ transforms under U(N). We have

$Z(k)\ Z^{+}(k) \sim$ 

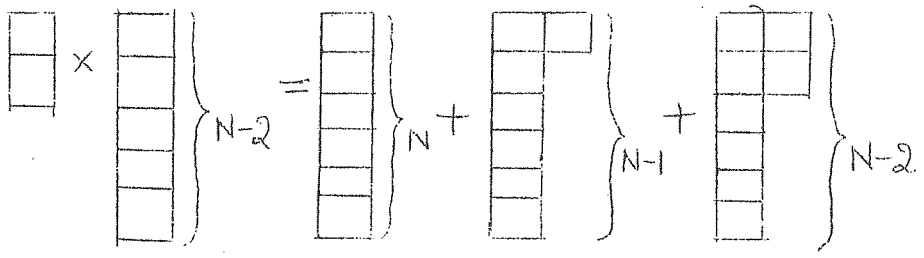
VC(7)

To find all the possible product representations we apply Littlewood's rules and consider only those representations which are allowed by the Pauli principle. These considerations limit us to only two-columned representations. To see how this process goes in general let us consider the reductions for one and two-body operators.

<u>k=1</u>



k=2



$$= [1^N] + [2, 1^{N-2}] + [2^2, 1^{N-4}]$$

Similarly for a k-body operator F(k) we get

$$F(k) \sim [1^k] \times [1^{N-k}]$$

$$= [1^N] + [2,1^{N-2}] + [2^2, 1^{N-4}] + \ldots + [2^{N-R}, 1^{2k-N}] \quad (k > \tfrac{N}{2})$$

VC(8a)

$$= [1^N] + [2,1^{N-2}] + [2^2,1^{N-4}] + \ldots + [2^k, 1^{N-2k}] \quad (k \leq \tfrac{N}{2})$$

VC(8b)

Thus for a k-body operator F(k) we get (k+1) different representations which we label as $[N-\nu, \nu]$ with $\nu = 0, 1, \ldots k$ and each representation occurs only once. In the labelling $[N-\nu, \nu]$, $(N-\nu)$ and ν denote the number of boxes in the first and the second column respectively. Note that $[N-\nu, \nu]$ is equivalent to $[2^\nu, 1^{N-2\nu}]$. We have then for F(k) the following reduction:

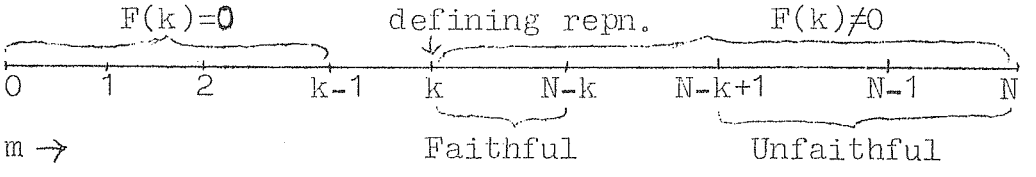
$$F(k) = \sum_{\nu=0}^{k} F^{\nu}(k)$$

where $F^{\nu}(k) \sim [N-\nu, \nu]$

VC(9)

The dimensionality of the representation $[N-\nu,\nu]$ is given by $d([N-\nu,\nu]) = \frac{(N-2\nu+1)}{(N+1)} \binom{N+1}{\nu}^2$. We have the useful relationship $\sum_{\nu=0}^{k} d([N-\nu,\nu]) = \binom{N}{k}^2$ which provides a check on the dimensionalities. In cases of interest we usually have only small values of k and large values of N. Then Eq.VC(8b) applies and the complexity of irreps appearing is limited by k and not by N.

We now consider the properties of the operators F(k) and $F^{\nu}(k)$. In order to find out what spaces support an irreducible operator i.e. those in which it has non-vanishing matrix elements, we first note that any k-body operator vanishes in m=0,1,....(k-1) particle spaces and is in general non-zero for $m \geq k$. We show in the following diagram the behaviour of a k-body operator F(k) when we represent it in the various m-particle subspaces:



VC(10)

Thus every m-particle space with $m \geq k$ gives a representation of F(k). However, not all of these representations are faithful. For example the m=N subspace is 1-dimensional and thus gives identity representations for all the operators that the space can support and therefore this will give an unfaithful representation.

In order to understand the nature of the supporting spaces let us first consider an operator of the type $G = \binom{n-\nu}{k-\nu} F(\nu)$ where n is the number operator $\sum_{i=1}^{N} A_i B_i$. $\binom{n-\nu}{k-\nu}$ is simply a polynomial in the number operator n and hence it is a U(N) scalar operator. Therefore $G=\binom{n-\nu}{k-\nu} F(\nu)$ transforms under U(N) exactly like the operator $F(\nu)$. Further, G is a pure k-body operator. This is because the binomial $\binom{n-\nu}{k-\nu}$ which is equal to $\frac{(n-\nu)(n-\nu-1)\ldots(n-k+1)}{(k-\nu)!}$ vanishes for $\nu \leq m \leq k-1$. Also by definition $F(\nu)$ vanishes for $m < \nu$. Therefore the product $G=\binom{n-\nu}{k-\nu} F(\nu)$ vanishes for $m \leq k-1$ and hence its particle rank can be $\geq k$. But the maximum particle rank of G is k which is just the sum of the ranks of the two factors $\binom{n-\nu}{k-\nu}$ and $F(\nu)$. We therefore get that G is a pure k-body operator with symmetry same as that of $F(\nu)$. Thus the operator $\binom{n-\nu}{k-\nu}$ when acting on an ν-body operator shifts the particle space in which the latter is defined without changing its unitary character i.e. if $F(\nu)$ has the symmetry

$[N-\nu\ ,\nu]$ then $\binom{n-\nu}{k-\nu}F(\nu)$ is a k-body operator with the same symmetry $[N-\nu\ ,\nu]$. In this way we can describe a k-body operator in terms of the set of subspaces which support it:

$$F(k) = \sum_{\nu=0}^{k} F^{\nu}(k) = \sum_{\nu=0}^{k} \binom{n-\nu}{k-\nu} f^{\nu}(\nu) \qquad \text{VC(11)}$$

where $f^{\nu}(\nu)$ has particle rank ν and symmetry $[N-\nu\ ,\nu]$. The operator $f^{\nu}(\nu)$ in Eq.VC(11) is irreducible and fully contracted in which we have factored out the number part $\binom{n-\nu}{k-\nu}$. As an example, we apply these considerations to one-body and two-body Hamiltonians when we obtain

$$h(1) = \sum_{\nu=0}^{1} \binom{n-\nu}{k-\nu} h^{\nu}(\nu)$$

$$= n\, h^{\nu=0}(\nu=0) + h^{\nu=1}(\nu=1)$$

VC(11a)

$$H(2) = \sum_{\nu=0}^{2} \binom{n-\nu}{2-\nu} H^{\nu}(\nu)$$

$$= \frac{n(n-1)}{2} H^{\nu=0}(0) + (n-1) H^{\nu=1}(1) + H^{\nu=2}(2)$$

VC(12)

$[N-\nu\ ,\nu]$ then $\binom{n-\nu}{k-\nu}F(\nu)$ is a k-body operator with the same symmetry $[N-\nu\ ,\nu]$. In this way we can describe a k-body operator in terms of the set of subspaces which support it:

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VC(11a)

$$H(2) = \sum_{\nu=0}^{2} \binom{n-\nu}{2-\nu} H^{\nu}(\nu)$$

$$= \frac{n(n-1)}{2} H^{\nu=0}(0) + (n-1) H^{\nu=1}(1) + H^{\nu=2}(2)$$

VC(12)

where $h^{\nu}(\nu)$ and $H^{\nu}(\nu)$ denote respectively the irreducible and fully contracted parts of h(1) and H(2) having the symmetry $[N-\nu, \nu]$ and particle rank ν. Comparing Eqs. VC(11a) and VC(12) it is clear that the $\nu=(0+1)$ part of H(2) behaves as an effective 1-body operator. Using this orthogonal decomposition for H(2) we get for the square of norm of H(2) in m-particle space:

$$
\begin{aligned}
&\| H(2) \|^2 \\
&= \langle H^{+}(2)\, H(2) \rangle^{m} \\
&= \left\langle \left[\sum_{\nu=0}^{2} \binom{n-\nu}{2-\nu} H^{\nu}(\nu) \right]^2 \right\rangle^{m} \\
&= \sum_{\nu=0}^{2} \left\langle \left\{ \binom{n-\nu}{2-\nu} H^{\nu}(\nu) \right\}^2 \right\rangle^{m} \\
&= \left\langle \left[\binom{n}{2} H^{\nu=0}(\nu=0) \right]^2 \right\rangle^{m} + \left\langle \left[(n-1) H^{\nu=1}(1) \right]^2 \right\rangle^{m} + \left\langle \left[H^{\nu=2}(2) \right]^2 \right\rangle^{m}
\end{aligned}
$$

In Eq.VC(13) cross terms like $\langle H^{\nu} H^{\nu'} \rangle^{m} \; (\nu \neq \nu')$ do not appear because they vanish due to the orthonormality of the tensors $H^{\nu}(\nu)$ (see Eq.VB(5)).

D. DECOMPOSITION OF OPERATORS ACCORDING TO THE SUBGROUP $U(m) \dot{+} U(N-m)$

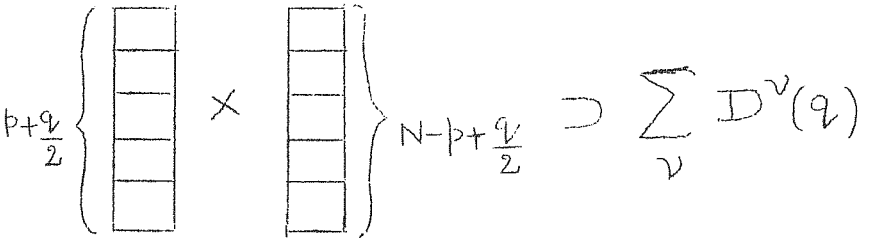
We described in the preceding section the decomposition

of a number conserving fermion operator according to the irreducible representations of the group U(N). We describe in this section the decomposition[5-8] of general fermion operators under the transformations of the direct sum subgroup $\sum_{i=1}^{\ell} U(N_i)$ of U(N). For this purpose we have to include into our discussion number non-conserving operators also. This done, the procedure for decomposition according to the subgroup is straightforward in that it proceeds along lines similar to the previous section.

We consider here an arbitrary division of the N-dimensional s.p.space of section C into ℓ s.p.subspaces with the i^{th} subspace having dimensionality N_i. Then the set of all unitary transformations operating within these independent subspaces considered simultaneously forms a subgroup of U(N), viz. the direct sum subgroup $\sum_{i=1}^{\ell} U(N_i)$. We shall call each subset of s.p.orbits $\{N_i\}$ a "Unitary orbit". The representations of the subgroup are characterized by a set of numbers $\vec{m} \equiv (m_1, m_2, \ldots m_\ell)$ with $\sum_{i=1}^{\ell} m_i = m$ where m_i is the number of particles in the i^{th} orbit.

The number conserving operators form only a restricted class of operators because in general the interactions do not preserve the number of particles in a unitary orbit. For example, the ordinary pairing Hamiltonian destroys

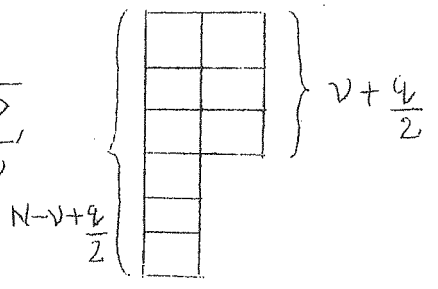
two particles in one j-orbit and creates two in another. It is therefore necessary to consider next the number non-conserving operators. To simplify the discussion, let us first consider a single unitary orbit and introduce general operators F(p,q) which make q particles in this orbit and where p denotes the particle rank. The operators $F(p,q) \in \left\{ A^{p+q/2} \; B^{p-q/2} \right\}$ with $-N \leq q \leq N$ and $p+q/2$ is integral. There are altogether 2^{4N} such operators. The number conserving operators all have q=0. To find the irreducible tensors contained in the product operator $A^{p+q/2} \; B^{p-q/2}$ we reduce it by applying Littlewood's rules and Pauli principle and obtain



$$\supset \sum_{\nu} D^{\nu}(q)$$

VD(1)

where



$$\sum_{\nu} D^{\nu}(q) = \sum_{\nu}$$

VD(2)

and $\frac{1}{2}|q| \leq \nu \leq \min(p,N-p)$ and $\nu + q/2$ integer. Here $D^{\nu}(q)$ denotes an irreducible representation and ν and q together label the representation. We get for the operator F,

$$F = \sum_{p,q} F(p,q) = \sum_{pq} \sum_{\nu} F^{\nu}(p,q) \qquad \text{VD(3)}$$

where q and ν are group labels. Now we factor out the number part in $F^{\nu}(p,q)$ as before and get the following decomposition equation for F(p,q):

$$F(p,q) = \sum_{\nu} \binom{n-\nu-q/2}{p-\nu} f^{\nu}(\nu,q) \qquad \text{VD(4)}$$

where the tensor $f^{\nu}(\nu,q)$ is irreducible and fully contracted. Since q is a group label we have the following orthogonality property for operators:

$$\left\langle F^{+}(p,q)\ G(p',q') \right\rangle^{m} = 0 \text{ unless } q = q' \qquad \text{VD(5)}$$

We have so far discussed the decomposition of a general operator F acting within a single unitary orbit. We now extend these notions to the case of many unitary orbits. Since the configuration spaces have a direct-product structure this extension becomes simple. We consider the division of the N-dimensional s.p. space into

ℓ s.p. subspaces each of dimension N_i. Thus $N = \sum_{i=1}^{\ell} N_i$. The labels p,q go over into ℓ -dimensional vectors

$$p \Rightarrow \vec{p} \equiv (p_1, p_2 \ldots . p_\ell)$$
$$q \Rightarrow \vec{q} \equiv (q_1, q_2 \ldots . q_\ell)$$

and the representations of operators under $\sum U(N_i)$ are labelled by a set of ℓ numbers $\vec{\nu} \equiv (\nu_1\ \nu_2\ \ldots .\ \nu_\ell)$, so that $F(p,q) \Rightarrow F(\vec{p},\vec{q})$ and $D^{\nu}(q) \Rightarrow D^{\vec{\nu}}(\vec{q})$. Then the decomposition equation for $F(\vec{p},\vec{q})$ is given by:

$$F(\vec{p},\vec{q}) = \sum_{\vec{\nu}} F^{\vec{\nu}}(\vec{p},\vec{q}) = \sum_{\vec{\nu}} \begin{pmatrix} \vec{n} - \vec{\nu} - \vec{q}/2 \\ \vec{p} - \vec{\nu} \end{pmatrix} f^{\vec{\nu}}(\vec{\nu},\vec{q})$$

VD(5a)

We discuss now a method[5-8] for obtaining explicit forms for the irreducible and fully contracted parts of any operator when decomposed according to the symmetries of U(N) and $\sum U(N_i)$. (Eqs.VC(11) and VD(5a)). For this purpose we introduce the notion of 'unitary scalar contraction' of an operator. We denote the operators for carrying out this contraction process by $D_{\pm}$ where D_+ is for boson operators and D_- for fermion operators. An operator F is boson like if it has even q and fermion like if q is odd.

The operators $D_{\pm}$ are defined as follows:

$$D_{\pm} F = \sum_{\mu=1}^{N} \left[A_\mu , \left[B_\mu , F \right]_{\mp} \right]_{\pm}$$

VD(6)

In Eq. VD(6) + on the right hand side denotes an anti-commutator and - a commutator. D is a contraction operator because D acting on F reduces its maximum particle rank by one. Moreover, $\sum_{\mu=1}^{N} A_\mu B_\mu$ is a unitary scalar operator and hence it cannot change the symmetry of F. The net result of D operation on F therefore is to reduce the maximum particle rank of F by one without changing its symmetry. It follows then that for a fully contracted, irreducible operator $\mathcal{F}^{\nu}(\nu, q)$, $D\mathcal{F}^{\nu}(\nu, q) = 0$. Thus if we have an irreducible operator $F^{\nu}(p,q)$ we can apply the D operator $(p - \nu)$ times on $F^{\nu}(p,q)$ and reduce it to its fully contracted form $\mathcal{F}^{\nu}(\nu, q)$.

We give here a few relevant relations[8] involving the D operator. For any two operators F and G,

1. $$D_{\pm}(FG) = (D_{+}(F))G + FD_{\pm}(G) \mp \sum_{\mu} \left\{ \left[A_\mu , F \right]_{-} \left[G , B_\mu \right]_{\mp} + \left[F, B_\mu \right]_{-} \left[G, A_\mu \right]_{\mp} \right\}$$

VD(7)

2. $$D(g(n)\ \mathcal{f}^{\nu}(q)) = g(n+1)(N-n-\nu+q/2)\ \mathcal{f}^{\nu}(q) - g(n)(N-2n+q)\ \mathcal{f}^{\nu}(q) - g(n-1)(n-\nu-q/2)\ \mathcal{f}^{\nu}(q) \qquad \text{VD(8)}$$

where $g(n)$ is any function of the number operator n.

3. For the operator $F^{\nu}(p,q)$ it can be shown that

$$DF^{\nu}(p,q) = (N+1-p-\nu)\ F^{\nu}(p-1,q) \qquad \text{VD(9)}$$

and

$$D^{r}\ F^{\nu}(p,q) = \sum_{\nu=\left|\frac{q}{2}\right|}^{p-r} r! \binom{N+r-p-\nu}{r} F^{\nu}(p-r,q) \qquad \text{VD(10)}$$

One can invert the expression in Eq. VD(10) to get the following expression for the irreducible, fully contracted tensor $\mathcal{f}^{\nu}(\nu,q)$:

$$\mathcal{f}^{\nu}(\nu,q) = \frac{1}{(p-\nu)!} \binom{N-2\nu}{p-\nu}^{-1} \sum_{t=p-\nu}^{p-\left|\frac{q}{2}\right|} \frac{(-1)^{t-p+\nu}}{(t-p+\nu)!} \binom{N-\nu-p+t+1}{t+\nu-p}^{-1} \times \binom{n-q/2-p+t}{t+\nu-p} D^{t}\ F\ (p,q) \qquad \text{VD(11)}$$

Thus, given any operator F(p,q) we can decompose it into its different unitary symmetry parts by repeated application of the D operator and obtain explicit form for each irreducible and completely contracted part using Eq.VD(11).

The extension of these ideas to the many orbit case is immediate. Here we have a contraction operator for each orbit and these operators act independently of each other. Hence the total contraction operator is just the product of these independent contraction operators. Also the various expressions in Eq.VD(9) - Eq.VD(11) go over to their vectorial form as in Eq.VD(5a).

E. UNITARY GROUP AND HARTREE-FOCK APPROXIMATION

We study in this section the question to what extent the high unitary rank parts of the interaction under U(N) get reduced to lower unitary rank parts under $\sum U(N_i)$. The particular subgroup we consider here is the direct sum subgroup U(m)+U(N-m) of U(N) which is generated by the HF procedure. Our main purpose is to find out the extent to which the HF procedure converts the two-body interaction term H(2) in the Hamiltonian into an effective one-body operator. In order to study this question we make use of a conversion ratio which provides us with a measure

of the efficiency of the HF procedure in converting the interaction into an effective one-body operator. We consider first the decomposition of the H(2) term into its different irreducible tensors according to the transformations of the subgroup $U(m)\dot{+}U(N-m)$ generated by the HF procedure. Next we derive a polynomial expression for the square of the norm of the total $(\vec{0}+\vec{1})$-unitary rank operator resulting from the HF decomposition of s.p. states.

We consider a set of N single-particle states in which m states are occupied. Let H denote the Hamiltonian of this system of m particles. In the HF picture the m-particle state is approximated by a Slater determinant Ψ_{HF} and further the m occupied states of Ψ_{HF} are such that Ψ_{HF} has lower energy than any other m-particle Slater determinant in the space. Let us refer to the space of m occupied s.p.states as the first unitary orbit and that of (N-m) unoccupied states as the second unitary orbit. Then the set of all unitary transformations which act independently and simultaneously in these two subspaces forms a subgroup of U(N) which is the direct sum subgroup $U(m)\dot{+}U(N-m)$. Thus we have

$$U(N) \supset U(m) \dot{+} U(N-m) \qquad \text{VE(1)}$$

The HF determinantal state is a unit dimensional configuration $\vec{m} \equiv (m_1, m_2) = (m, 0)$ where m_1 and m_2 are the number of particles in orbits 1 and 2 respectively. The HF procedure selects, from the family of different direct sum subgroups corresponding to different two-orbit partitioning of the N s.p. space, that subgroup which gives the lowest energy for the configuration $\vec{m} \equiv (m, 0)$. We next proceed to consider the tensor decomposition of H(2) under U(N) and also under its direct sum subgroup U(m)+U(N-m).

Under U(N) (see Eq.VC(9)), H(2) decomposes into the following irreps:

$$H(2) = \sum_{\nu=0}^{2} H^{\nu}(2)$$

$$= H^{\nu=0}(2) + H^{\nu=1}(2) + H^{\nu=2}(2) \qquad \text{VE(2)}$$

Under U(N), the $\nu = (0+1)$ part of H(2) is the effective one-body operator (see also Eqs.VC(11a) and VC(12)). The question how much of the total two-body interaction H(2) is in its lower unitary rank components $\nu = 0$ and $\nu = 1$ under U(N) has already been studied[8]. It is found that in 0d-1s and 0f-1p shells with realistic two-body interactions the norm of $H^{\nu=2}(2)$ part of the interaction is very much larger than the norm of $H^{\nu=1}(2)$ which means that H(2) has a large irreducible part under U(N). The same result is borne out by

our calculations which we shall describe later in Sections F and G. Hence if no appreciable reduction of the irreducible part of H(2) is to be found under U(N), one might consider a finer analysis of H(2) under the subgroup $U(m)\dot{+}U(N-m)$ to see whether in that case it looks essentially like a one-body operator. We want to find out how much of the U(N) irreducible $H^{\nu=2}(2)$ part gets converted into a lower unitary rank operator under $U(m)\dot{+}U(N-m)$ which is the direct sum subgroup generated by the HF procedure. Now the $H^{\nu=2}(2)$ which is irreducible under U(N) does not remain so under the subgroup transformation but breaks up into $\vec{\nu}=(0+1+2)$ parts under the subgroup. Therefore let us consider the decomposition of H(2) into its irreducible representations under this subgroup:

$$H(2) = \sum_{\vec{\nu}=0}^{2} H_{\vec{\nu}}(2)$$

$$= H_{\vec{\nu}=0}(2) + H_{\vec{\nu}=1}(2) + H_{\vec{\nu}=2}(2) \qquad \text{VE(3)}$$

where we denote the irreducible tensors with respect to the subgroup by subscripts $\vec{\nu}$. Under $U(m)\dot{+}U(N-m)$ the effective one-body operator is $(H_{\vec{\nu}=0}(2) + H_{\vec{\nu}=1}(2))$. This is the total effective one-body operator one obtains when a HF calculation is done. This one-body operator receives

contributions from all the three U(N) symmetry parts of H(2). We can depict the decompositions under U(N) and the subgroup schematically as follows:

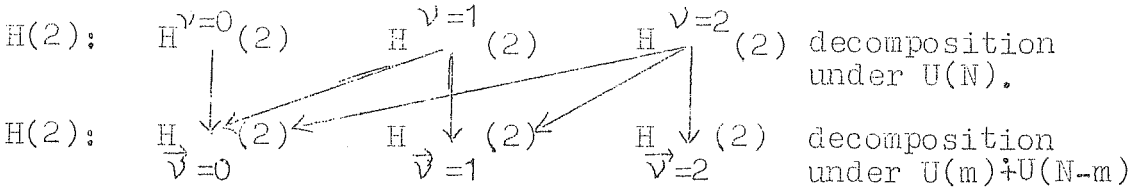


Fig. V-1

It is clear that a given unitary rank operator under U(N) breaks up into its lower unitary rank operators under the subgroup decomposition. The question we wish to study now is how much of the high unitary rank ($\nu = 2$) part of H(2) gets converted into lower unitary rank parts $\vec{\nu}=(0+1)$ under U(m)+U(N-m). This will tell us how efficient the HF procedure is in reducing the two-body interaction into an effective one-body operator. We now define a ratio which will measure for us this efficiency factor

$$R = \frac{\left\langle \left[H_{\vec{\nu}=0}^{(2)} + H_{\vec{\nu}=1}^{(2)} \right]^2 \right\rangle^m - \left\langle \left[H^{\nu=0}(2) \right]^2 \right\rangle^m - \left\langle \left[H^{\nu=1}(2) \right]^2 \right\rangle^m}{\left\langle \left[H^{\nu=2}(2) \right]^2 \right\rangle^m}$$

where in the numerator the first term is the square of the norm (in the m-particle space) of subgroup $\vec{\nu}=(0+1)$ part of H(2). From this term we subtract the squares of norms of $\nu = 0$ and $\nu = 1$, U(N) irreducible symmetry parts of H(2). Therefore the numerator gives us the square of the size of subgroup $\vec{\nu} = (0+1)$ operator coming only from $H^{\nu=2}(2)$. The denominator is the square of the norm of $H^{\nu=2}(2)$. Thus the ratio R tells us how much of the U(N) irreducible operator $H^{\nu=2}(2)$ gets converted into subgroup $\vec{\nu}=(0+1)$-rank operator when a HF calculation is done.

We now consider the decomposition of H(2) under U(m)+U(N-m) which must be done before we can proceed to evaluate the ratio R. To recall, we have a set of N single-particle states of which m are occupied. We refer to the set of m occupied states as the 1st orbit and denote all the operators in this orbit by subscript 1. The (N-m) unoccupied states will be referred to as the 2nd orbit and all the operators in this orbit will be subscripted by 2. We have

$$H(2) = \frac{1}{4} \sum_{ijk\ell} \langle ij \mid v \mid kl \rangle \; A_i A_j B_l B_k \qquad \text{VE(5)}$$

where the A's and B's are the single-particle creation

and destruction operators respectively and obey the well-known anticommutation rules (see Eq.IIB(2)). We rewrite H(2) as:

$$\begin{aligned} H(2) = {} & A_1A_1B_1B_1 + A_1A_1B_1B_2 + A_1A_1B_2B_2 \\ & + A_1A_2B_1B_1 + A_1A_2B_1B_2 + A_1A_2B_2B_2 \\ & + A_2A_2B_1B_1 + A_2A_2B_1B_2 + A_2A_2B_2B_2 \end{aligned} \qquad \text{VE(6)}$$

In Eq.VE(6), $A_1A_1B_1B_1 = \frac{1}{4} \sum_{ijk\ell \in 1} \langle ij|v|k\ell\rangle\, A_iA_jB_1B_k$,

$A_1A_2B_1B_2 = \frac{1}{4} \sum_{\substack{i\ell \in 1 \\ jk \in 2}} \langle ij|v|k\ell\rangle\, A_iA_jB_1B_k$ and so on.

Thus we have written H(2) as a sum of nine sets of operators of which one acts in orbit 1 only and another in orbit 2 only and the rest act between these orbits. We now rewrite each term in the Eq.VE(6) using a different notation

$$H(p_1p_2;q_1q_2) = A_1^{p_1+q_1/2}\, A_2^{p_2+q_2/2}\, B_1^{p_1-q_1/2}\, B_2^{p_2-q_2/2}$$

VE(7)

We get

$$H(2) = H(20;00) + H(3/2\ 1/2;\ 1\text{-}1) + H(11;2\text{-}2) + H(3/2\ 1/2;\ \text{-}11) + H(11;00) + H(1/2\ 3/2;\ 1\text{-}1) + H(11;\text{-}22) + H(1/2\ 3/2;\ \text{-}11) + H(02;\ 00) \qquad \text{VE(8)}$$

For instance, the operator $A_1A_2B_1B_2$ in Eq.VE(6) gives $p_1+q_{1/2} = 1$, $p_2+q_{2/2} = 1$, $p_1-q_{1/2} = 1$ and $p_2-q_{2/2}=1$ from which we get $p_1=1$, $p_2=1$, $q_1=0$ and $q_2=0$. Thus $A_1A_2B_1B_2 = H(p_1p_2,\ q_1q_2) = H(11;00)$. The notation used in Eq.VE(7) is an extension to the case of two unitary orbits of the notation used in Eq.VD(3) wherein we considered only one unitary orbit. We now consider the reduction under $U(m) \dot{+} U(N\text{-}m)$ of various terms on the right side of Eq.VE(8). Following Eq.VD(3) we write

$$H(p_1p_2;\ q_1q_2) = \sum_{\nu_1\nu_2} H^{\nu_1\nu_2}(p_1p_2;\ q_1q_2) \qquad \text{VE(9)}$$

where $H^{\nu_1\nu_2}(p_1p_2;q_1q_2)$ denotes an irreducible representation with respect to the subgroup $U(m)+U(N\text{-}m)$. ν_1,ν_2 together with q_1,q_2 completely specify the representation. The labels ν_1 and ν_2 denote the irreducible symmetries of the term $H^{\nu_1\nu_2}(p_1p_2,q_1q_2)$ in the orbits 1 and 2 respectively. Thus this term behaves as a tensor

of rank ν_1 in orbit 1 and as a tensor of rank ν_2 in orbit 2. Further, for ν we have

$$\tfrac{1}{2}\,|q_i| \leq \nu_i \leq \min\,(p_i,\ N_i - p_i)$$

and $\nu_i + q_{i/2}$ integer. $\quad i = 1,2.$

VE(10)

Now we use the expansion in Eq.VE(9) for all the terms on the right side of Eq.VE(8). This gives us 20 irreducible representations for H(2).We get[8]

$$H(2) = \sum_{p_1 q_1 \nu_1} \sum_{p_2 q_2 \nu_2} H^{\nu_1\,\nu_2}(p_1 p_2; q_1 q_2)$$

$$= H^{00}(20;00)+H^{00}(11;00)+H^{00}(02;00)$$

$$+ H^{10}(20;00)+H^{10}(11;00)+H^{01}(11;00)+H^{01}(02;00)$$

$$+H^{\frac{1}{2}\frac{1}{2}}(3/2\ 1/2;1\text{-}1)+H^{\frac{1}{2}\frac{1}{2}}(3/2\ 1/2;\text{-}11)+H^{\frac{1}{2}\frac{1}{2}}(1/2\ 3/2;1\text{-}1)$$

$$+H^{\frac{1}{2}\frac{1}{2}}(1/2\ 3/2;\ \text{-}11)$$

$$+H^{20}(20;00)+H^{11}(11;00)+H^{11}(11;2\text{-}2)+H^{11}(11;\text{-}22)$$

$$+H^{02}(02;00)+H^{3/2\ 1/2}(3/2\ 1/2;1\text{-}1)+H^{3/2\ 1/2}(3/2\ 1/2;\text{-}11)$$

$$+H^{1/2\ 3/2}(1/2\ 3/2;1\text{-}1)+H^{1/2\ 3/2}(1/2\ 3/2;\ \text{-}11)$$

VE(11)

In Eq.VE(11) the first three terms which have $\vec{\nu}_1 + \vec{\nu}_2 = 0$ are scalar with respect to the subgroup, behaving respectively as $\binom{n_1}{2}$, $n_1 n_2$ and $\binom{n_2}{2}$; we denote them together by $H_0(2)$. The next eight terms having $\vec{\nu}_1 + \vec{\nu}_2 = 1$ are the effective traceless one-body terms which we label together as $H_1(2)$. The last 9 terms with $\vec{\nu}_1 + \vec{\nu}_2 = 2$ are irreducible two-body terms and give zero on contraction. We are interested here in the complete $\vec{\nu} = (0+1)$ part of H(2) which is the effective one-body operator coming from the U(m)+U(N-m) decomposition of H(2). We write

$$
\begin{aligned}
H'(2) &= H_{\vec{\nu}=0}(2) + H_{\vec{\nu}=1}(2) \\
&= H^{00}(20;00) + H^{00}(11;00) + H^{00}(02;\ 00) \\
&+ H^{10}(20;00) + H^{10}(11;00) + H^{01}(11;00) + H^{01}(02;00) \\
&+ H^{\frac{1}{2}\frac{1}{2}}(3/2\ 1/2;\ 1\text{-}1) + H^{\frac{1}{2}\frac{1}{2}}(3/2\ 1/2;\ -11) + H^{\frac{1}{2}\frac{1}{2}}(1/2\ 3/2;\ 1\text{-}1) \\
&+ H^{\frac{1}{2}\frac{1}{2}}(1/2\ 3/2;\ -11)
\end{aligned}
$$

VE(12)

Thus H'(2) is of particle rank 2, and has unitary irreducible symmetry $\vec{\nu} = (0+1)$ with respect to the group U(m)+U(N-m). It is the total effective one-body operator one obtains when a general decomposition is made of N s.p. into m occupied states and (N-m) unoccupied ones. We now

proceed to evaluate the norm of $H'(2)$ in m-particle spaces which are defined by the underlying HF s.p. basis. For this special case of the HF decomposition of s.p.states there is a simplification in that the underlined terms in Eq.VE(12) do not contribute to the norm of $H'(2)$. This comes about because the contribution of these two terms to the norm of $H'(2)$ involves essentially the matrix elements of the Hamiltonian between 0p-0h and 1p-1h states and these are zero in the case of HF decomposition. We digress here a little to show why we have considered $H'(2)$ instead of the HF s.p. Hamiltonian h itself to study the question about the conversion efficiency of the HF procedure. First we note that not all the terms of $H'(2)$ contribute to the HF s.p. Hamiltonian h. The HF s.p. Hamiltonian in general is of the form

$$h = H(1) + D_1\ H(2) \qquad \text{VE(13)}$$

where $H(1)$ is the pure single-particle term and $D_1\ H(2)$ is the one-body potential derived from the two-body $H(2)$ by contracting $H(2)$ over all the occupied s.p. states (orbit no.1). The definition of the contraction operator D_1 here is the same as in Eq.VD(6) but now the contraction is restricted to occupied states only. Further, in the HF procedure the occupied states are such that they give

minimum energy for the system. It can be shown that the terms of H(2)(see Eq.VE(8)) that survive when the HF procedure and contraction are carried out are H(20;00) and H(11;00) only. We write these two terms together as $H_{HF}(2)$.

$$H_{HF}(2) = H(20;00) + H(11;00) \qquad \text{VE(14)}$$

Then

$$h = H(1) + D_1 H_{HF}(2) \qquad \text{VE(15)}$$

Decomposing $H_{HF}(2)$ into its irreducible symmetry parts under $U(m)\dot{+}U(N-m)$ we get

$$H_{HF}(2) = H^{00}(20;00)+H^{10}(20;00)+\underline{H^{20}(20;00)}$$
$$+H^{00}(11;00)+H^{01}(11;00)+\underline{H^{10}(11;00)}+\underline{H^{11}(11;00)} \qquad \text{VE(16)}$$

Since under contraction the unitary rank ν of the operator does not change, but its particle rank p decreases by unity (see Eq.VD(9)), we find that when D_1 acts on $H_{HF}(2)$ only those symmetries ν which satisfy $\nu \leq p$ are allowed

in $D_1 H_{HF}(2)$. Hence the underlined terms in Eq.VE(16) do not contribute to $D_1 H_{HF}(2)$. Therefore the HF s.p. Hamiltonian h takes the following form:

$$h = H(1) + D_1 H_{HF}(2)$$

$$= H(1) + D_1 \left[H^{00}(20;00) + H^{10}(20;00) + H^{00}(11;00) + H^{01}(11;00) \right]$$

VE(17)

The unitary tensor structure of the HF s.p. Hamiltonian h is now clear. We see that $H_{HF}(2)$ which has the same unitary structure as the HF s.p. Hamiltonian h forms only a part of $H'(2)$ (Eq.VE(12)) which is the total effective one-body operator one can have in the HF decomposition. Thus there are other terms in $H'(2)$ which have the same unitary tensor character as $H_{HF}(2)$ and from a mathematical point of view the norm of $H_{HF}(2)$ would not be a sound prescription as a measure. This is because the HF decomposition

$$H(2) = H_{HF}(2) + (H(2) - H_{HF}(2))$$

VE(18)

is not an orthogonal decomposition of H(2) and when norms

are taken, there is no guarantee that condition no.3 in Eq.VB(1) will always be satisfied. It may therefore lead to contradictory situations in which the ratio R (Eq.VE(4)) becomes greater than unity. Hence the norm of $H_{HF}(2)$ as a measure for our purpose is only of suspicious value. We therefore study the Hamiltonian $H'(2)$.

To return to Eq.VE(12), each term on the right side there is unitarily irreducible but contractible. Now we write each term as a product of two parts, one part that is purely a number operator and the other one the unitarily irreducible, fully contracted part. To do this, we have only to extend the decomposition equation of Eq.VD(4) to the case of two unitary orbits remembering that the group transformations in these two orbits act independently of each other. We get for each term $H^{\nu_1\nu_2}(p_1p_2;q_1q_2)$

$$H^{\nu_1\nu_2}(p_1p_2;q_1q_2) = \begin{pmatrix} n_1-\nu_1-q_1/2 \\ p_1-\nu_1 \end{pmatrix} \begin{pmatrix} n_2-\nu_2-q_2/2 \\ p_2-\nu_2 \end{pmatrix} \times$$

$$\times f^{\nu_1\nu_2}(p_1p_2;q_1q_2)$$

VE(19)

where n_1 and n_2 are number operators in orbits 1 and 2 respectively. $f^{\nu_1\nu_2}(p_1p_2;q_1q_2)$ is the completely reduced, fully contracted part of $H^{\nu_1\nu_2}(p_1p_2;q_1q_2)$. It behaves as a tensor of rank ν_1 in the 1st unitary orbit and of rank ν_2 in the 2nd orbit. Note that $f^{\nu_1\nu_2}(p_1p_2;q_1q_2)$ $\equiv f^{\nu_1\nu_2}(\nu_1\ \nu_2;\ q_1q_2)$. Using Eq.VE(19) in Eq.VE(12) we obtain for $H'(2)$

$$H'(2) = \binom{n_1}{2} f^{00}(20;00)+n_1n_2 f^{00}(11;00)+\binom{n_2}{2} f^{00}(02;00)$$
$$+(n_1-1) f^{10}(20;00)+n_2 f^{10}(11;00)+n_1 f^{01}(11;00)$$
$$+(n_2-1) f^{01}(02;00) + n_2 f^{\frac{1}{2}\frac{1}{2}}(1/2\ 3/2;\ 1\text{-}1)$$
$$+(n_2-1) f^{\frac{1}{2}\frac{1}{2}}(1/2\ 3/2;\ \text{-}11) \qquad \text{VE(20)}$$

In order to obtain explicit forms for the irreducible operators $f^{\nu_1\nu_2}(p_1p_2;q_1q_2)$ appearing in Eq.VE(20) we make use of expression given in Eq.VD(11) for the single unitary orbit case. In the case of two unitary orbits we have two contraction operators D_1 and D_2 which act respectively in orbits 1 and 2 and are independent. We have for $H'(2)$

$$H'(2) = \frac{1}{4} \sum_{ijkl} \langle ij|v|kl\rangle \; A_i A_j B_l B_k$$

and we carry out first the contraction in orbit 1 (that is, the 1st orbit is completely filled with N_1 particles while the 2nd orbit is empty and the contraction is over the filled 1st orbit), to get the explicit expressions for the fully reduced and contracted tensors in orbit 1. We show the procedure here by working out in detail the explicit form for $\mathcal{F}^{00}(20;00)$. Consider the term

$$T = \binom{n_1}{2} \mathcal{F}^{00}(20;00) \qquad \text{VE(21)}$$

which is the first term on the right side of Eq.VE(20). Now because of the factor $\binom{n_1}{2}$ in T, T will be non-zero only in the 1st orbit and it will be zero in all other cases. Hence we can write

$$T = \frac{1}{4} \sum_{ijkl \in 1} \langle ij|\, v \,|\, kl\rangle \; A_i A_j B_l B_k \qquad \text{VE(22)}$$

where i,j,k,l are s.p. states in the 1st orbit only. Now applying the contraction operator D_1 on T we get

$$D_1 \; T = D_1 \; \binom{n_1}{2} \mathcal{F}^{00}(20;00) \qquad \text{VE(23)}$$

Following Eq.VD(6) we have for $D_1 T$

$$D_1 T = \sum_{\mu \in 1} \left[A_\mu , \left[B_\mu , T \right]_- \right]_+$$

VE(24)

where μ runs over the states in 1st orbit only. Using Eq.VE(22) for T in Eq.VE(24) we get

$$D_1 T = \sum_{\mu \in 1} \left[A_\mu , \left[B_\mu , \frac{1}{4} \sum_{ijk\ell \in 1} \langle ij|V|k\ell\rangle A_i A_j B_\ell B_k \right]_- \right]_+$$

After expanding the commutators and using the fermion anticommutation rules we obtain

$$D_1 T = \sum_{ijk \in 1} \langle ij|V|kj\rangle A_i B_k$$

$$= \sum_{ik \in 1} \epsilon_{ik} A_i B_k$$

VE(25)

where

$$\epsilon_{ik} = \sum_{j \in 1} \langle ij|V|kj\rangle$$

VE(26)

Applying again the D_1 operator in Eq.VE(25) we obtain

$$D_1^2 T = \sum_{i \in 1} \epsilon_{ii}$$

$$= N_1 \overline{e_1}$$

VE(27)

where

$$\overline{e_1} = \frac{1}{N_1} \sum_{i \in 1} \epsilon_{ii}$$

On the other hand, we have from Eq.VE(23)

$$D_1 T = D_1 \binom{n_1}{2} f^{00}(20;00)$$

$$= (N_1 - 1) n_1 f^{00}(20;00)$$

VE(28)

which follows from Eq.VD(8). Using again Eq.VD(8) we get

$$D_1^2 T = D_1 \left[(N_1 - 1)\, n_1 f^{00}(20;00) \right] = (N_1 - 1)\, N_1 f^{00}(20;00)$$

Now we have $D_1^2 T = N_1 (N_1 - 1)\, f^{00}(20;00) = N_1 \overline{e_1}$

therefore

$$f^{00}(20;00) = \left(\frac{1}{N_1 - 1}\right) \overline{e_1}$$

VE(29)

In order to obtain compact and physically understandable expressions for the other irreducible fully contracted tensors we define various single-particle quantities as follows:

We have a set of N s.p. states of which N_1 states are in the 1st orbit and N_2 are in the 2nd orbit. We denote the s.p.states of the 1st orbit by $\lambda, \mu, \cdots$ and those of the 2nd orbit by a,b,c... and arbitrary s.p.states by i,j,k,... . Then we define with respect to contraction in the 1st orbit the following single-particle quantities:

For a general one-body operator ϵ its matrix element between s.p.states i and j is defined as

$$\epsilon_{ij} = \sum_{\lambda=1}^{N_1} \langle i\lambda | v | j\lambda \rangle \qquad \text{VE(30)}$$

A. Average s.p.quantities

$$\overline{e_1} = \frac{1}{N_1} \sum_{\lambda \in 1} \epsilon_{\lambda\lambda} \qquad \text{VE(31)}$$

$$\overline{e_2} = \frac{1}{N_2} \sum_{a \in 2} \epsilon_{aa} \qquad \text{VE(32)}$$

B. Traceless s.p.quantities

$$e'_\lambda = \epsilon_{\lambda\lambda} - \overline{e_1} \qquad \text{VE(33)}$$

$$e'_a = \epsilon_{aa} - \overline{e}_2 \qquad \text{VE(34)}$$

In terms of these s.p.quantities we obtain the following expressions:

$$f^{00}(20;00) = \frac{1}{(N_1-1)}\,\overline{e}_1 \qquad \text{VE(35)}$$

$$f^{00}(11;00) = \frac{1}{N_1}\,\overline{e}_2 \qquad \text{VE(36)}$$

$$f^{10}(20;00) = \frac{1}{(N_1-2)}\left[\sum_{\substack{\lambda\neq\mu \\ \epsilon 1}} \epsilon_{\lambda\mu} A_\lambda B_\mu + \sum_{\lambda} e'_\lambda n_\lambda\right] \qquad \text{VE(37)}$$

$$f^{01}(01;00) = \frac{1}{N_1}\left[\sum_{\substack{a\neq b \\ \epsilon 2}} \epsilon_{ab} A_a B_b + \sum_{a} e'_a n_a\right] \qquad \text{VE(38)}$$

Here the number operators $n_\lambda = \sum_{\lambda\epsilon 1} A_\lambda B_\lambda$ and $n_a = \sum_{a\epsilon 2} A_a B_a$. In order to obtain the explicit forms for the remaining $f^{\nu_1\nu_2}(p_1p_2;q_1q_2)$ in Eq.VE(20) we have to consider next the contraction with respect to the 2nd orbit by the operator D_2. The situation in this case is that the 1st orbit is empty and the 2nd orbit of N_2 s.p.states

is now completely filled. We contract the two-body interaction over the N_2 occupied states of the 2nd orbit using D_2 and obtain the following expressions for the irreducible and fully contracted tensors with respect to orbit 2.

$$f^{00}(02;00) = \frac{1}{(N_2-1)} \bar{\tilde{e}}_1 \qquad \text{VE(39)}$$

$$f^{10}(11;00) = \frac{1}{N_2}\left[\sum_{\substack{\lambda\neq\mu \\ \in 1}} \tilde{\epsilon}_{\lambda\mu} A_\lambda B_\mu + \sum_\lambda \tilde{e}_{\lambda'} n_\lambda\right] \qquad \text{VE(40)}$$

$$f^{01}(02;00) = \frac{1}{(N_2-2)}\left[\sum_{a\neq b \in 2} \tilde{\epsilon}_{ab} A_a B_b + \sum_a \tilde{e}'_a n_a\right] \qquad \text{VE(41)}$$

$$f^{\frac{1}{2}\frac{1}{2}}(1/2\ 3/2;1\text{-}1) = \frac{1}{(N_2-1)} \sum_{\substack{\lambda\in 1 \\ a\in 2}} \tilde{\epsilon}_{\lambda a} A_\lambda B_a \qquad \text{VE(42)}$$

$$f^{\frac{1}{2}\frac{1}{2}}(1/2\ 3/2;\ \text{-}11) = \frac{1}{(N_2-1)} \sum_{\substack{\lambda\in 1 \\ a\in 2}} \tilde{\epsilon}_{a\lambda} A_a B_\lambda \qquad \text{VE(43)}$$

In the above expressions the various s.p.quantities are defined with respect to contraction in the 2nd orbit as follows: We consider a general one-body operator which is defined through its matrix elements as follows:

$$\tilde{\epsilon}_{ij} = \sum_{a\in 2} \langle ia|v|ja\rangle$$

VE(44)

where i,j are arbitrary s.p.states and the summation is over all the filled N_2 states of the 2nd orbit.

A. Average s.p. quantities

$$\bar{\tilde{e}}_1 = \frac{1}{N_2} \sum_{a\in 2} \tilde{\epsilon}_{aa}$$

VE(45)

$$\bar{\tilde{e}}_2 = \frac{1}{N_1} \sum_{\lambda\in 1} \tilde{\epsilon}_{\lambda\lambda}$$

VE(46)

B. Traceless s.p. quantities

$$\tilde{e}'_\lambda = \tilde{\epsilon}_{\lambda\lambda} - \bar{\tilde{e}}_2$$

VE(47)

$$\tilde{e}'_a = \tilde{\epsilon}_{aa} - \bar{\tilde{e}}_1$$

VE(48)

To obtain the expression for the square of the norm of $H'(2)$ we have to consider the product $H'^{+}(2)\, H'(2)$. Since the decomposition of $H'(2)$ in Eq.VE(20) is an orthogonal one we need not consider the cross terms

between $\vec{\nu} = 0$ and $\vec{\nu} = 1$ terms which appear in the product $H'^{+}(2)\, H'(2)$ as their averages in m-particle spaces vanish according to

$$\left\langle f^{\nu_1\nu_2}(p_1p_2;q_1q_2)\, f^{\nu_1'\nu_2'}(p_1'p_2';q_1'q_2') \right\rangle^{m} = \delta_{\nu_1\nu_1'}\,\delta_{\nu_2\nu_2'}\,\delta_{q_1q_1'}\,\delta_{q_2q_2'}$$

VE(49)

Using Eq.VE(20) for $H'(2)$ and remembering Eq.VE(49) we obtain for the product $H'^{+}(2)\, H'(2)$ the following expression:

$$\begin{aligned}
H'^{+}(2)\, H'(2) = {} & \left[\binom{n_1}{2} f^{00}(20;00)\right]^{+}\left[\binom{n_1}{2} f^{00}(20;00)\right] \\
& + \left[n_1n_2\, f^{00}(11;00)\right]^{+}\left[n_1n_2\, f^{00}(11;00)\right] \\
& + \left[\binom{n_2}{2} f^{00}(02;00)\right]^{+}\left[\binom{n_2}{2} f^{00}(02;00)\right] \\
& + \left\{\left[\binom{n_1}{2} f^{00}(20;00)\right]^{+}\left[n_1n_2\, f^{00}(11;00)\right]\right. \\
& \left. + \left[n_1n_2\, f^{00}(11;00)\right]^{+}\left[\binom{n_1}{2} f^{00}(20;00)\right]\right\} \\
& + \left\{\left[n_1n_2\, f^{00}(11;00)\right]^{+}\left[\binom{n_2}{2} f^{00}(02;00)\right]\right. \\
& \left. + \left[\binom{n_2}{2} f^{00}(02;00)\right]^{+}\left[n_1n_2\, f^{00}(11;00)\right]\right\}
\end{aligned}$$

$$
\begin{aligned}
&+\left\{\left[\binom{n_1}{2}\ f^{00}(20;00)\right]^{+}\left[\binom{n_2}{2}\ f^{00}(02;00)\right]\right.\\
&\qquad\left.+\left[\binom{n_2}{2}\ f^{00}(02;00)\right]^{+}\left[\binom{n_1}{2}\ f^{00}(20;00)\right]\right\}\\
&+\left[(n_1-1)\ f^{10}(20;00)\right]^{+}\left[(n_1-1)\ f^{10}(20;00)\right]\\
&+\left[n_1\ f^{01}(11;00)\right]^{+}\left[n_1\ f^{01}(11;00)\right]\\
&+\left[n_2\ f^{10}(11;00)\right]^{+}\left[n_2 f^{10}(11;00)\right]\\
&+\left[(n_2-1)\ f^{01}(02;00)\right]^{+}\left[(n_2-1)\ f^{01}(02;00)\right]\\
&+\left[n_2\ f^{\frac{1}{2}\frac{1}{2}}(1/2\ 3/2;1\text{-}1)\right]^{+}\left[n_2\ f^{\frac{1}{2}\frac{1}{2}}(1/2\ 3/2;\ 1\text{-}1)\right]\\
&+\left[(n_2-1)\ f^{\frac{1}{2}\frac{1}{2}}(1/2\ 3/2;\text{-}11)\right]^{+}\left[(n_2-1)\ f^{\frac{1}{2}\frac{1}{2}}(1/2\ 3/2;\text{-}11)\right]\\
&+\left\{\left[(n_1-1)\ f^{10}(20;00)\right]^{+}\left[n_2\ f^{10}(11;00)\right]\right.\\
&\qquad\left.+\left[n_2\ f^{10}(11;00)\right]^{+}\left[(n_1-1)\ f^{10}(20;00)\right]\right\}\\
&+\left\{\left[(n_2-1)\ f^{01}(02;00)\right]^{+}\left[n_1\ f^{01}(11;00)\right]\right.\\
&\qquad\left.+\left[n_1\ f^{01}(11;00)\right]^{+}\left[(n_2-1)\ f^{01}(02;00)\right]\right\}
\end{aligned}
$$

VE(50)

We next consider the expression for the average value of $H'^{+}(2)\,H'(2)$ in m-particle space. We have from Eq.VB(7),

$$\left\langle H'^{+}(2)\,H'(2)\right\rangle^{m}$$

$$= \binom{N-m}{u_2+1} \sum_{s=0}^{u_1} (-1)^{s-u_1} \binom{N-s}{u_2+1}^{-1} \binom{m-s-1}{u_1-s} \binom{m}{s} \left\langle H'^{+}(2)H'(2)\right\rangle^{s}$$

$$+ \binom{m}{u_1+1} \sum_{s=0}^{u_2} (-1)^{s-u_2} \binom{N-s}{u_1+1}^{-1} \binom{N-m-s-1}{u_2-s} \binom{N-m}{s} \left\langle H'^{+}(2)H'(2)\right\rangle^{N-s}$$

where $u_1+u_2=u-1$, u being the maximum particle rank in $H'^{+}(2)\,H'(2)$. In the present case $u=4$, and we take $u_1=u/2$, $u_2=(u-2)/2$ for 'maximum economy' (see Sec.VB). Then $u_1=2$, $u_2=1$. With this choice the average of $H'^{+}(2)\,H'(2)$ can be expressed in terms of its averages $\left\langle H'^{+}(2)\,H'(2)\right\rangle^{s}$ in s=0,1,2 particle spaces and s=0,1 hole spaces. Since $H'^{+}(2)\,H'(2)$ has minimum particle rank 2, its average obviously vanishes in 0 and 1 particle spaces. Therefore the average of $H'^{+}(2)\,H'(2)$ is given in terms of its averages $\left\langle H'^{+}(2)\,H'(2)\right\rangle^{s}$ in s=1, N-1, and N particle spaces only. Thus we get:

$$\left\langle H'^{+}(2)\, H'(2)\right\rangle^{m} = \binom{N-m}{2}\binom{N-2}{2}^{-1}\binom{m}{2}\left\langle H'^{+}(2)H'(2)\right\rangle^{2}$$

$$+\binom{m}{3}\binom{N-1}{3}^{-1}(N-m)\left\langle H'^{+}(2)\, H'(2)\right\rangle^{N-1}$$

$$-\binom{m}{3}\binom{N}{3}^{-1}(N-m-1)\left\langle H'^{+}(2)\, H'(2)\right\rangle^{N}$$

VE(51)

For the explicit form of $\left\langle H'^{+}(2)\, H'(2)\right\rangle^{m}$ we therefore need to obtain the expressions for the averages of $H'^{+}(2)\, H'(2)$ in 2, N-1, and N particle spaces. This involves going through a mass of algebra but the procedure is straightforward. We do not give here these details but present only the final expression that results for the square of the norm of $H'(2)$ in m-particle space:

$$\left\langle H'^{+}(2)\, H'(2)\right\rangle^{m}$$

$$= \binom{N-m}{2}\binom{N-2}{2}^{-1}\binom{m}{2}\binom{N}{2}^{-1}\times$$

$$\times\left\{\frac{N_1}{2(N_1-1)}\bar{e}_1^{\,2} + \frac{N_2}{N_1}\bar{e}_2^{\,2} + \frac{N_2}{2(N_2-1)}\bar{\bar{e}}_1^{\,2}\right.$$

$$+\frac{1}{(N_1-2)}\left[\sum_{\lambda\neq\mu}\epsilon^2_{\mu\lambda}+\sum_{\lambda}e'^2_{\lambda}\right]$$

$$+\frac{1}{N_1}\left[\sum_{a\neq b}\epsilon^2_{ab}+\sum_{a}e'^2_{a}\right]$$

$$+\frac{1}{N_2}\left[\sum_{\lambda\neq\mu}\tilde{\epsilon}^2_{\lambda\mu}+\sum_{\lambda}\tilde{e}'^2_{\lambda}\right]$$

$$+\frac{1}{(N_2-2)}\left[\sum_{a\neq b}\tilde{\epsilon}^2_{ab}+\sum_{a}\tilde{e}'_{a}\right]$$

$$+\frac{1}{(N_2-1)^2}\left[4(N_2-1)+(N_1-1)\right]\sum_{\lambda a}\tilde{\epsilon}^2_{\lambda a}$$

$$+\frac{(N-1)}{(N_2-1)^2}\sum_{a\lambda}\tilde{\epsilon}^2_{a\lambda}\Bigg\}$$

$$+\binom{m}{3}\binom{N-1}{3}^{-1}(N-m)\frac{1}{N}\Bigg\{$$

$$\frac{1}{4}\left[N_1(N_1-2)^2+N_2N_1^2\right]\bar{e}_1^2$$

$$+\left[\frac{(N_1-1)^2N_2^2}{N_1}+N_2(N_2-1)^2\right]\bar{e}_2^2$$

$$+\frac{1}{4}\left[N_1N_2^2+N_2(N_2-2)^2\right]\bar{\tilde{e}}_1^2$$

$$+\left[(N_1-1)(N_1-2)N_2+N_1N_2(N_2-1)\right]\overline{e}_1\overline{e}_2$$

$$+\frac{1}{2}\left[N_1N_2(N-4)\right]\overline{e}_1\overline{\tilde{e}}_1$$

$$+\left[(N_1-1)N_2^2+N_2(N_2-1)(N_2-2)\right]\overline{e}_2\overline{\tilde{e}}_1$$

$$+\sum_\lambda e_\lambda'^2+\sum_a e_a'^2$$

$$+\sum_\lambda e_\lambda'^2+\sum_{\lambda\neq\mu}\tilde{\epsilon}^2_{\lambda\mu}$$

$$+\sum_a \tilde{e}_a'^2+\sum_{a\neq b}\tilde{\epsilon}^2_{ab}$$

$$+\frac{N_2^2}{(N_2-1)^2}\sum_{\lambda a}\tilde{\epsilon}^2_{\lambda a}$$

$$+\frac{(N_2-2)^2}{(N_2-1)^2}\sum_{\lambda a}\tilde{\epsilon}^2_{\lambda a}$$

$$+2\left[\sum_\lambda e_\lambda'\tilde{e}_\lambda'+\sum_{\lambda\neq\mu}\epsilon_{\lambda\mu}\tilde{\epsilon}_{\mu\lambda}\right]$$

$$+2\left[\sum_a e_a'\tilde{e}_a'+\sum_{a\neq b}\epsilon_{ab}\tilde{\epsilon}_{ba}\right]$$

$$- \binom{m}{3}\binom{N}{3}^{-1}(N-m-1)\Big\{$$

$$\frac{N_1^2}{4}\bar{e}_1^2 + N_2^2\bar{e}_2^2 + \frac{N_2^2}{4}\bar{\bar{e}}_1^2$$

$$+ N_1N_2\bar{e}_1\bar{e}_2 + \frac{N_1N_2}{2}\bar{e}_1\bar{\bar{e}}_1$$

$$+ N_2^2\bar{e}_2\bar{\bar{e}}_1\Big\}$$

VE(52)

The various single-particle quantities $\bar{e}_1, \bar{\bar{e}}_1$ etc. have already been defined in Eqs.VE(30) - VE(34) and VE(44)-VE(48). Using Eq. VE(52) for the square of the norm of subgroup $\vec{\nu}=(0+1)$ rank operator we can evaluate the conversion ratio R in Eq.VE(4) for a given HF decomposition of s.p.states knowing, of course, also the norms of $\nu = 0,1,2$ rank parts of H(2) decomposed with respect to U(N).

F. NUMERICAL RESULTS AND DISCUSSION:Of-1p SHELL

We discuss in this section our calculations and results for norms of different irreducible unitary tensor parts of H(2) and also the evaluation of conversion ratio

R for some 0f-1p shell nuclei.

For our calculations we have taken the full 0f-1p shell of $0f_{7/2}$, $1p_{3/2}$, $0f_{5/2}$ and $1p_{1/2}$ s.p.levels. For the sake of simplicity we have taken these levels to be degenerate at zero energy and thus the Hamiltonian H in our calculations consists of only the two-body interaction term H(2). The two-body interaction H(2) used here is the Kuo-Brown effective interaction in the 0f-1p shell modified by McGrory, Wildenthal and Halbert (MWH)[9] in an attempt to optimize the agreement with the experimental spectra of Ca isotopes.

First, we consider the norms of the different symmetry parts of H(2) decomposed according to the U(N) group. These U(N) norms we have calculated using the computer code of Chang[8]. We show these results in Table V-1 where in the first column m is the total number of particles of the nucleus. The next three columns show the squares of norms of $\nu = 0$, $\nu = 1$ and $\nu = 2$ rank parts of H(2) resulting from its decomposition under the group U(N). We see that the $\nu = 0$ part of the interaction is the largest of the three symmetry parts in almost all the cases. This means interaction is predominantly U(N) scalar. In the nonscalar part it is largely $\nu = 2$, the $\nu = 1$ part

being smaller than $\nu = 2$ by orders of magnitude. Considering the propagation formula of these norms we find that the $H^{\nu=1}(2)$ part would increase much faster with m compared to $H^{\nu=2}(2)$. This is because the $\nu = 1$ and $\nu = 2$ parts of H(2) propagate in m-particle spaces according to different polynomials involving the number operator, the $\nu = 1$ coefficient increasing much faster than the $\nu = 2$ coefficient with increase in m. Thus one would expect that the $\nu = 1$ part of H(2) will become dominant as m increases. This does not happen with the MWH interaction because the norm $||H^{\nu=1}||_{m=1}$ is very small.

We now discuss the results of norms under the subgroup decomposition of H(2). We have considered here only the N=Z even even nuclei in the 0f-1p shell. For each nucleus the calculation involves two steps. In the first step, we carry out a HF calculation for the nucleus under the assumption of axial symmetry for the intrinsic state. We do this for both prolate and oblate deformations and then select the lowest of these two HF solutions. In the second step, we consider the entire set of single-particle wave functions and energies of the lowest HF solution. Using these s.p.wave functions and energies we evaluate the various s.p.average quantities defined in Eqs.VE(30)-VE(34) and Eqs.VE(44)-VE(48). We next evaluate the square of the

norm of $H'(2)$ using the expression in Eq.VE(52). We show the results of our calculations in Tables V-1 and V-2. In Table V-1, the fifth column shows the deformation of the lowest HF solution the letters P,O,S denoting respectively the prolate, the oblate and the spherical solutions. The last three columns show the squares of the norms of $\vec{\nu}=0$, $\vec{\nu}=1$ and $\vec{\nu}=2$ rank tensors resulting from the decomposition of H(2) according to the irreducible representations of the subgroup $U(m)\dot{+}U(N-m)$. From these results we see that the $\vec{\nu}=0$ part of the interaction is the largest component. The size of the $\vec{\nu}=1$ part is still very small compared to the sizes of other components. Comparing the norms of parts of H(2) under U(N) and $U(m)\dot{+}U(N-m)$ we find that the subgroup norms are only slightly larger than the U(N) norms. First we observe that the scalar components dominate the whole scene in both U(N) and subgroup decompositions. The increase in the $\nu=0$ component when we go to the subgroup decomposition is not much. Next, the ratio of the squares of norms of $\nu=1$ parts viz. $||H_{\vec{\nu}=1}||^2 / ||H^{\nu=1}||^2$ is about 9 for m=4 and it decreases to about 1.7 in the middle of the shell (m=20). In short, the decomposition picture of the interaction does not change much when we go from U(N) to its direct-sum subgroup $U(m)\dot{+}U(N-m)$ generated by the

HF method. In Table V-2 we show in column 5 the ratio R (see Eq.VE(4)) evaluated for different nuclei. This ratio is the difference between numbers in columns 2 and 3 divided by the number in column 4. The norm square of subgroup $H^{\nu=(0+1)}(2)$ (column 2) is seen to be only slightly larger than the norm square of $H^{\nu=(0+1)}(2)$ with respect to U(N). The ratio R turns out to be around 5% for most of the nuclei studied. This shows that the HF procedure converts apparently only a small part of the irreducible $\nu=2$ part of the two-body interaction into a one-body like operator. In other words, under the transformations of the subgroup generated by the HF decomposition of s.p.states the two-body interaction term does not seem to be very much reducible into an effective one-body operator. Since we do not know the optimum value of the ratio R that can be achieved for this particular interaction in this particlar space (by making a general decomposition of the N s.p. states into m occupied states and (N-m) unoccupied ones) we do not know whether or not this 'small' value of 5% for R is already near the optimum value of R. The problem of finding out that subgroup U(m)+U(N-m) which optimizes the ratio R remains to be tackled.

Since the square of norm of an operator is the average of the square of the operator over the entire m-particle space, it contains information about the behaviour of the operator from all regions of the spectrum. Hence the measure it provides for the size of the operator is always a "global" one. Therefore the ratio R which is a ratio of the norms tells us about the goodness of the s.p.basis from a global standpoint. Thus the ratio in the case of HF decomposition of s.p.states does not tell about the latter's goodness in any particular energy region of the spectrum. The small value we get for R essentially means that the HF s.p. basis is not uniformly good over the entire spectrum. It does not say anything about the HF in the ground state domain.

G. NUMERICAL RESULTS AND DISCUSSION: Od-1s SHELL

We now discuss our calculations and results for norms of different irreducible symmetry parts of H(2) and also the evaluation of conversion ratio R for some Od-1s shell nuclei.

As before the Hamiltonian in our calculations does not have the pure one-body part and thus we have here a pure two-body term H(2) for the Hamiltonian and a set of

s.p.levels consisting of $0d_{5/2}$, $1s_{1/2}$ and $0d_{3/2}$ levels degenerate at zero energy. For H(2) we have used three different interactions viz. the Preedom-Wildenthal interaction (PW)[10], the Schematic interaction (see Chapter IV, Section C) and the K+12FP interaction[11].

First, let us consider the results of U(N) norm calculations using the three interactions. These are shown in Tables V-3, V-5 and V-7. We show in these tables the same quantities as were shown in Table V-1. We see from these results that in the case of PW and K+12FP interactions $H^{\nu=0}(2)$ is the dominant part. The K+12FP $\nu=0$ part is much larger than the PW $\nu=0$ part throughout the 0d-1s shell. Next, we see that the $\nu=1$ norm in the PW interaction is larger than the $\nu=1$ norm in the K+12FP interaction. This $\nu=1$ component has an appreciable magnitude (for all m shown) in the case of PW interaction and in the K+12FP case it is smaller by almost an order of magnitude. If we next look at the square of norms of the $\nu=2$ part of H(2) we find that it is larger than the $\nu=1$ part in both the interactions. The PW $\nu=2$ part has a somewhat larger size than its K+12FP counterpart. In short, the $\nu=0$ strength is dominant in both the interactions and the size of $\nu=1$ part in PW is appreciable and is larger than the K+12FP $\nu=1$

part. In both the interactions there is a large part which is irreducible.

The U(N) norms with the schematic interaction are shown in Table V-5. The decomposition picture here is strikingly different. We notice that the $\nu=0$ is not the dominating component and it has a size comparable to that of $\nu=1$ part in almost throughout the shell. As regards the $\nu=2$ part it is much larger than $\nu=0$ and $\nu=1$ parts in almost every case. Thus this interaction is dominantly of the higher unitary symmetry type ($\nu=2$) whereas in the PW and K+12FP interactions the scalar strength dominates.

We now consider the norms of H(2) decomposed under the subgroup $U(m)\dot{+}U(N-m)$. These results are shown in Table V-3 up to Table V-8 for the three different interactions. The same quantities as were shown in Tables V-1 and V-2 are shown here also. From Table V-3 we see that the $\nu'=0$ continues to be the dominant part of the PW interaction when one goes from U(N) decomposition to the $U(m)\dot{+}U(N-m)$ decomposition. The norm of $\vec{\nu}=1$ is still small although it increases by an order of magnitude when we go from the beginning to the middle of the shell. If we compare the norms of the $\vec{\nu}=0$ and $\vec{\nu}=1$ parts with respect to U(N) and $U(m)\dot{+}U(N-m)$ we find that in most cases under

the subgroup decomposition each of these parts is only slightly larger than what it is under U(N). Consequently the size of the effective one-body operator increases but slightly when we go from the group U(N) to its subgroup $U(m)\dot{+}U(N-m)$ (Table V-4, columns 2 and 3). The difference in the squares of the norms of this operator under the two groups seems to attain a maximum in the middle of the shell ($\sim$ 11 MeV^2). Let us consider next the efficiency ratio R shown in the last column in Table V-4. This ratio is seen to be small for all m listed, its value ranging from 6.7% (m=8) to 25%(m=20). This means that there is no substantial reduction of the higher unitary symmetry part of the interaction i.e. $H^{\nu=2}(2)$ into its lower symmetry parts under the subgroup $U(m)\dot{+}U(N-m)$ when a HF calculation is done.

The results of subgroup norms with the K+12FP interaction are shown in Tables V-7 and V-8. It is clear from these results that under subgroup decomposition a large part of the strength resides in the $\vec{\nu}$ =0 component. The $\vec{\nu}$ =1 part is by itself quite small and has not changed much compared to its U(N) counterpart. The ratio R shown in Table V-8 is small indeed in all the cases shown. It is maximum at 9% for m=16. A 9% reduction of the U(N)

irreducible $H^{\nu=2}(2)$ part into $\vec{\nu}=(0+1)$ part under $U(m)+U(N-m)$ indicates that the HF s.p.basis is by no means a good basis considered over the entire energy range. In the case of the results of the subgroup norms for the Schematic interaction (Tables V-5 and V-6) the $\vec{\nu}=0$ and $\vec{\nu}=1$ norms are comparable and are much smaller than the $\vec{\nu}=2$ norm which as in U(N) decomposition, again holds the show. If we next look at the ratio R in Table V-6 we see that it is quite small in all the cases.

It is clear from all this discussion that the HF decomposition is not effective in reducing the higher unitary symmetry parts of the two-body interaction into its lower unitary symmetry parts. Further the smallness of the ratio R essentially means that the HF s.p.basis as a universal basis is not a good basis although it may be good in the ground state region.

The conversion ratio R together with U(N) norms can be used to serve as a good guide in answering the question which interactions are suitable for using in HF calculations. Given two interactions we can say that the interaction which has appreciable U(N) irreducible part (i.e. $H^{\nu=2}(2)$) and which gives a larger value for

the ratio R on the whole is better suited for using in HF calculations than the other one. Of course this is not a very precise indicator but it does serve as a guide in answering the above stated question. From this point of view, comparing the values of the ratio R and norms of $H^{\nu=2}(2)$ part for the three interactions in Tables V-4, V-6 and V-8 we see that the Preedom-Wildenthal (PW) interaction is marginally better than the other two interactions.

TABLE V-1

Norms of unitary symmetry parts of H(2) decomposed according to the groups U(N) and U(m)+U(N-m) (Hartree-Fock) for N=Z even-even nuclei in 0f-1p shell. H(2): McGrory-Wildenthal-Halbert interaction

	Square of norm of $H^{\nu}(2)$ under U(N)			HF solution	Square of norm of $H_{\vec{\nu}}(2)$ under U(m)+U(N-m)		
m	$\nu=0$	$\nu=1$	$\nu=2$		$\vec{\nu}=0$	$\vec{\nu}=1$	$\vec{\nu}=2$
4	3.9003	0.0126	8.05	P	4.168	0.0964	7.69
8	84.940	0.1224	29.58	P	85.74	0.8695	28.03
12	471.93	0.3968	53.13	P	474.28	0.9933	50.18
16	1560.12	0.8434	70.54	0	1563.4	1.3670	66.74
20	3911.15	1.4096	76.88	0	3914.0	2.3885	72.98
24	8253.1	1.9829	70.54	P	8256.3	2.5317	66.84
28	15480.3	2.3911	53.13	0	15482.7	3.0542	50.13
32	26653.9	2.4015	29.58	0	26654.6	3.3283	27.88
36	43001.0	1.7219	8.05	0	43001.2	1.9812	7.55

TABLE V-2

Norms of unitary symmetry parts of H(2) decomposed according to the group U(N) and U(m)+U(N-m) (Hartree-Fock) for N=Z even-even nuclei in 0f-1p shell. H(2): McGrory- Wildenthal-Halbert interaction

m	Square of norm of $H^{\vec{\nu}}(2)$ w.r.t. U(m)+U(N-m) $\vec{\nu}=(0+1)$	Square of norm of $H^{\nu}(2)$ w.r.t. U(N) $\nu=(0+1)$	$\nu=2$	Ratio R (%)
4	4.2654	3.9129	8.05	4.37
8	86.611	85.062	29.58	5.23
12	475.28	472.33	53.13	5.55
16	1564.8	1560.97	70.54	5.42
20	3916.4	3912.5	76.88	5.07
24	8258.8	8255.1	70.54	5.24
28	15485.7	15482.7	53.13	5.64
32	26658.0	26656.3	29.58	5.74
36	43003.2	43002.7	8.05	6.21

TABLE V-3

Norms of unitary symmetry components of H(2) decomposed according to the groups U(m)+U(N-m) (Hartree-Fock)and U(N) for N=Z even-even nuclei in 0d-1s shell.

H(2): Preedom-Wildenthal interaction

	Square of norm of $H^{\nu}(2)$ under U(N)			HF solu-	Square of norm of $H_{\vec{\nu}}(2)$ under U(m)+U(N-m)		
m	$\nu=0$	$\nu=1$	$\nu=2$	tion	$\vec{\nu}=0$	$\vec{\nu}=1$	$\vec{\nu}=2$
4	21.22	1.29	26.49	P	22.83	1.72	24.55
8	462.21	11.24	78.09	0	465.75	12.94	72.85
12	2568.11	31.22	101.24	0	2575.37	35.20	90.01
16	8489.64	51.61	78.09	0	8505.00	41.51	72.83
20	21283.05	51.75	26.49	0	21288.05	53.49	19.79

TABLE V-4

Norms of unitary symmetry component of H(2) decomposed according to the groups U(m)+U(N-m) (Hartree-Fock) and U(N) for N=Z even-even nuclei in 0d-1s shell.

H(2): Preedom-Wildenthal interaction

m	Square of norm of $H_{\vec{\nu}}(2)$ under U(m)+U(N-m) $\vec{\nu}=(0+1)$	Square of norm of $H^{\nu}(2)$ under U(N) $\nu=(0+1)$	$\nu=2$	Ratio R (%)
4	24.5666	22.5144	26.49	7.74
8	478.690	473.453	78.09	6.70
12	2610.57	2599.34	101.24	11.09
16	8546.51	8541.25	78.09	6.73
20	21341.5	21334.8	26.49	25.29

TABLE V-5

Norms of unitary symmetry components of H(2) decomposed according to the groups $U(m)\dot{+}U(N-m)$ (Hartree-Fock) and U(N) for N=Z even-even nuclei in 0d-1s shell.

H(2): Schematic interaction

m	Square of norm of $H^{\nu}(2)$ under U(N) $\nu=0$	$\nu=1$	$\nu=2$	HF solution	Square of norm of $H_{\vec{\nu}}(2)$ under $U(m)\dot{+}U(N-m)$ $\vec{\nu}=0$	$\vec{\nu}=1$	$\vec{\nu}=2$
4	0.1381	0.5464	115.02	P	4.6016	1.2001	109.90
8	3.0067	4.7603	339.03	0	13.781	6.631	326.38
12	16.705	13.224	439.53	P	34.524	15.60	419.33
16	55.224	21.858	339.03	P	65.820	24.40	325.89
20	138.44	21.919	115.02	0	143.50	23.88	108.00

TABLE V-6

Norms of unitary symmetry components of H(2) decomposed according to the groups U(m)+U(N-m) (Hartree-Fock) and U(N) for N=Z eve-even nuclei in 0d-1s shell.
H(2): Schematic interaction

m	Square of norm of $H^{\vec{\nu}}(2)$ under U(m)+U(N-m) $\vec{\nu}$=(0+1)	Square of norm of $H^{\nu}(2)$ under U(N) ν=(0+1)	ν= 2	Ratio R (%)
4	5.8017	0.6845	115.02	4.44
8	20.4122	7.7670	339.03	3.72
12	50.1240	29.929	439.53	4.59
16	90.2224	77.083	339.03	3.87
20	167.396	160.36	115.02	6.11

TABLE V-7

Norms of unitary symmetry components of H(2) decomposed according to the groups U(m)+U(N-m) (Hartree-Fock) and U(N) for N=Z even-even nuclei in 0d-1s shell.
H(2): K+12FP interaction

m	Square of norm of $H^{\nu}(2)$ under U(N) ν=0	ν=1	ν=2	HF solution	Square of norm of $H_{\vec{\nu}}(2)$ under U(m)+U(N-m) $\vec{\nu}$=0	$\vec{\nu}$=1	$\vec{\nu}$=2
4	38.280	0.1821	25.34	P	39.804	0.4614	23.53
8	833.65	1.5868	74.69	0	836.93	2.5176	70.48
12	4631.8	4.4082	96.83	P	4638.6	5.1538	89.33
16	15312.0	7.2864	74.69	0	15314.0	12.027	67.89
20	38386.3	7.3066	25.34	S	38394.3	0.008	24.64

TABLE V-8

Norms of unitary symmetry components of H(2) decomposed according to the groups U(m)+U(N-m) (Hartree-Fock) and U(N) for N=Z even-even nuclei in 0d-1s shell.

H(2): K+12FP interaction

m	Square of norm of $H_{\vec{\nu}}(2)$ under U(m)+U(N-m)	Square of norm of $H^{\nu}(2)$ under U(N)		Ratio R (%)
	$\vec{\nu}=(0+1)$	$\nu=(0+1)$	$\nu=2$	
4	40.265	38.462	25.342	7.11
8	839.45	835.24	74.694	5.63
12	4643.7	4636.2	96.836	7.74
16	15326.0	15319.2	74.694	9.10
20	38394.3	38393.6	25.342	2.76

REFERENCES FOR CHAPTER V

1. J.B.French, Physics Letters, 26B, 75 (1967).
2. J.B.French, "Spectral Distributions in Nuclei", Dacca Lectures (1967).
3. J.B. French, "Spectral Distributions in Nuclei in Nuclear Structure", North Holland Publishing Company, Amsterdam (1967).
4. C.M. Vincent, Phys. Rev. 163, 1044 (1967).
5. F.S. Chang, J.B. French and T.H. Thio, Annals of Physics, 66, 137 (1971).
6. J.C. Parikh, Article on "Group Symmetries in Nuclear Structure" to appear in Advances in Nuclear Physics.
7. J.B. French, Proc. Summer Institute of Theoretical Physics, Chandigarh, May 1971, Vol.III.
8. F.S. Chang, Ph.D. Thesis, University of Rochester (1970).
9. J.B. McGrory, B.H. Wildenthal and E.C. Halbert, Phys. Rev.C2, 186 (1970).
10. M. Preedom and B.H. Wildenthal, Phys. Rev. C6,1633 (1972).
11. E.C. Halbert et al, Advances in Nuclear Physics, Vol.4, Chapter 6, edited by M. Baranger and E. Vogt, Plenum Press (1971).
12. M. Hamermesh, Group Theory (Pergamon Press Ltd.,London, 1962).

CHAPTER VI

SUMMARY AND FUTURE PROSPECTS

To sum up, we have studied in this thesis two distinct topics. The first topic deals with the goodness of Hartree-Fock states and also with the variational method based on the minimization of energy variance for obtaining Slater determinants. In the second topic we have studied the decomposition of fermion operators under unitary groups and the norms of these operators in spectroscopic spaces.

In the first place, we have studied the goodness of HF states by evaluating their widths. The width of a state provides us with a measure of the departure of the state from an exact eigenstate of the nuclear system in the model space. We have evaluated the widths of HF states of some light spherical nuclei using realistic two-body interactions. We find that the HF states have large widths which implies that the HF single Slater determinantal description is inadequate.

Besides studying the goodness of HF states we have also investigated in detail a new variational method wherein we minimize the energy variance of a Slater determinant

instead of its energy as is done in the conventional HF method. We have derived the equations for determining the self-consistent set of single particle orbits using the new variational procedure. We have applied this method to some light spherical nuclei. We find that the new procedure yields determinants which are close to the HF determinants. We have also calculated perturbation theory corrections for both kinds of determinants viz. the HF and the minimum variance determinant to estimate the correlation effects. A comparative study of the properties of the Slater determinants obtained from the two variational procedures has also been made. Further, we have also studied the goodness of deformed HF states of some N=Z even even nuclei in the 0d-1s major shell.

The second major topic dealt with in this thesis is about the structure of fermion operators and spaces. We have studied here the question to what extent the HF procedure converts the two-body interaction into an effective one-body operator. For this purpose we require two things. First, we need a proper classification scheme for operators in which we can carry out an orthogonal decomposition of them. Secondly, we need proper measures or norms for the sizes of operators so that we can study their behaviour in spectroscopic spaces and also make a

comparative study of them. In our study we have used the group theoretic classification for operators the relevant groups being unitary groups in spectroscopic spaces. More precisely, we have here a set of N single-particle states in which m particles are distributed. We have classified the two-body interaction according to the irreducible symmetries of the unitary group U(N) and its direct sum subgroup $U(m)\dot{+}U(N-m)$. The subgroup here is the one generated by the HF decomposition of s.p. space into m occupied and (N-m) unoccupied states. We have studied here the question to what extent the irreducible tensor part of the two-body interaction H(2) under U(N) is converted into an effective one-body operator under the subgroup $U(m)\dot{+}U(N-m)$ supplied by the HF procedure. As already said, for our purpose we need also suitable norms for the sizes of operators in m particle spaces. We have used here the Euclidean norm as a proper measure for the size of an operator. We have derived a polynomial expression for the square of the norm of the effective one-body operator which results when the two-body interaction is classified under the subgroup generated by the HF procedure. Next a quantity called conversion ratio is defined in terms of norms of different symmetry parts of the interaction decomposed according to U(N) and

U(m)+U(N-m). This ratio tells us to what extent the two-body interaction has been converted into an effective one-body operator when a HF calculation is done. It further indicates in a global sense how good is the HF single-particle basis. This ratio has been evaluated for the HF solutions of some N=Z even even nuclei both in 0f-1p and 0d-1s shells using realistic two-body interactions. Our studies reveal that this conversion is quite small which implies that a large part of the two-body interaction is still irreducible under the subgroup generated by the HF procedure and that the HF s.p. basis is not a good universal basis.

Finally a few suggestions for future investigations which emerge from these studies may be indicated here:

(a) Our study of widths has shown that single Slater determinantal description of exact eigenstates of the Hamiltonian is inadequate. One way of improving the determinantal energy and wave function is to correct them in perturbation theory by including 1ph and 2ph correlations as we did in Chapter III. A better approach which is nonperturbative is through an elementary application of Lanczos algorithm. This involves the evaluation of moments of the Hamiltonian H in the determinantal state Ψ . If we restrict

ourselves to the model space consisting of 0ph, 1ph and 2ph states then we can reduce the energy eigenvalue problem to the diagonalization of a 2x2 matrix whose elements are given in terms of the first three moments of the Hamiltonian in the state Ψ . This method provides an exact solution of the system in the model space.

(b) The energy variance minimization method described in this thesis may be modified to include constraints. If one can minimize the energy variance of a determinant at a given energy then one has the best s.p. basis (in the sense of minimum width) at that energy. This will be helpful in the study of level densities etc.

(c) As already mentioned in Chapter III, it will be interesting to investigate whether the expectation values $\langle \Psi | H^p | \Psi \rangle$ $(p > 2)$ where Ψ is a Slater determinant, also become minimum the neighbourhood of the HF minimum.

(d) The expression for the square of the norm of effective one-body operator which we have derived in Chapter V can be easily extended for the general case by including all those terms which were zero

for the HF decomposition. Maximization of this norm may then provide a s.p. basis in which the Hamiltonian looks essentially like a (0+1)-body operator. This is admittedly hard to carry out but it will be quite interesting if one can achieve it. As a first step in tackling this problem one can study it in simple situations where the s.p.basis states are defined by just one-parameter,as for example, in the Nilsson model where a single deformation parameter defines the single particle states.